

Supporting Information

Efficient One-Pot Quinoline Derivative Synthesis from Acetophenone and Allyl Alcohols

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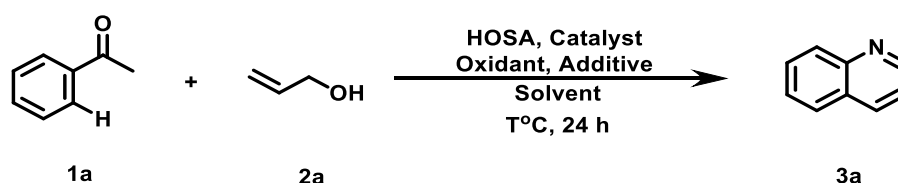
1. General Information

Catalytic reactions were carried out in Schlenk tubes using pre-dried glassware. Various products (quinoline) were synthesized according to previously described procedures. Commercially available reagents, such as Catalysts and substrates 1 were purchased from Energy Chemical, and used without purification unless otherwise noted. Column chromatography purification was performed using 200–300 mesh silica gel. NMR spectra were mostly recorded for ¹H NMR at 400 MHz and for ¹³C NMR at 101 MHz. CDCl₃ and DMSO-D₆ were used as solvents. Chemical shifts were referenced relative to residual solvent signal (CDCl₃: ¹H NMR: δ 7.26 ppm, ¹³C NMR: δ 77.16 ppm; DMSO-D₆: ¹H NMR: δ 2.50 ppm, ¹³C NMR: δ 39.52 ppm). The following abbreviations are used to describe peak patterns where appropriate: br = broad, s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet. Coupling constants (J) are reported in Hertz (Hz). HRMS was performed on Agilent Technologies 6224 TOF LC/MS apparatus (ESI).

2. Experimental Section

2.1. Preliminary optimization of reaction conditions

Table S1. Reaction condition screening of 3a.

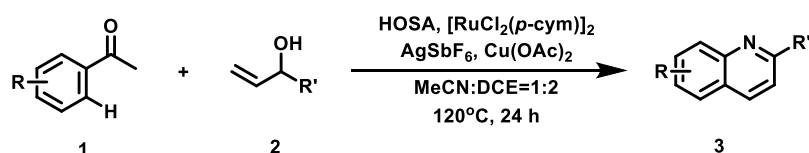


Entry	Catalyst	Oxidant	Solvent	T(°C)	Additive	Yield (%) ^b
1	[Cp*RhCl ₂] ₂	AgSbF ₆	MeCN:HFIP=1:2	120°C	Cu(OAc) ₂	30
2	[RuCl ₂ (<i>p</i> -cymene)] ₂	AgSbF ₆	MeCN:HFIP=1:2	120°C	Cu(OAc) ₂	45
3	[Cp*IrCl ₂] ₂	AgSbF ₆	MeCN:HFIP=1:2	120°C	Cu(OAc) ₂	NR
4	[Cp*RuCl ₂] ₂	AgSbF ₆	MeCN:HFIP=1:2	120°C	Cu(OAc) ₂	NR
5	Cp*CoCOI ₂	AgSbF ₆	MeCN:HFIP=1:2	120°C	Cu(OAc) ₂	NR
6	[RuCl ₂ (<i>p</i> -cymene)] ₂	Ag ₂ O	MeCN:HFIP=1:2	120°C	Cu(OAc) ₂	NR
7	[RuCl ₂ (<i>p</i> -cymene)] ₂	Ag ₂ CO ₃	MeCN:HFIP=1:2	120°C	Cu(OAc) ₂	26
8	[RuCl ₂ (<i>p</i> -cymene)] ₂	AgSbF ₆	MeCN:DMF=1:2	120°C	Cu(OAc) ₂	NR
9	[RuCl ₂ (<i>p</i> -cymene)] ₂	AgSbF ₆	MeCN:MeOH=1:2	120°C	Cu(OAc) ₂	48
10	[RuCl ₂ (<i>p</i> -cymene)] ₂	AgSbF ₆	MeCN:DCE=1:2	120°C	Cu(OAc) ₂	85
11	[RuCl ₂ (<i>p</i> -cymene)] ₂	AgSbF ₆	MeCN:DCE=1:2	100°C	Cu(OAc) ₂	36
12	[RuCl ₂ (<i>p</i> -cymene)] ₂	AgSbF ₆	MeCN:DCE=1:2	110°C	Cu(OAc) ₂	77
13	[RuCl ₂ (<i>p</i> -cymene)] ₂	AgSbF ₆	MeCN:DCE=1:2	130°C	Cu(OAc) ₂	83
14	[RuCl ₂ (<i>p</i> -cymene)] ₂	AgSbF ₆	MeCN:DCE=1:2	120°C	AcOH	30
15	[RuCl ₂ (<i>p</i> -cymene)] ₂	AgSbF ₆	MeCN:DCE=1:2	120°C	NaOAc	45
16	[RuCl ₂ (<i>p</i> -cymene)] ₂	AgSbF ₆	MeCN:DCE=1:2	120°C	CsOAc	50

^aReaction conditions: **1** (0.5 mmol), **2** (0.75 mmol), HOSA (1.0 mmol), Catalyst (5.0 mol %), Oxidant (1.0 mmol), Additive (2 mmol), in the solvent (3.0 mL) for 24 h. ^bYields of isolated products.

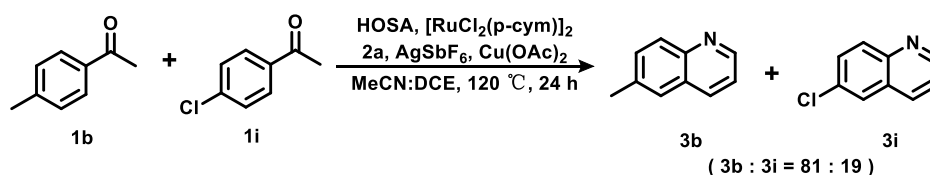
2.2. Synthesis and characterization of products 3

2.2.1 Preparation of quinoline products (Method A)



A reaction tube (10 mL) with magnetic stir bar was charged with compound **1** (0.5 mmol, 1.0 equiv), HOSA (1.0 mmol) and 1 mL MeCN. Then the mixture was stirred at room temperature for 3 h. TLC (PE: EA= 4:1) showed that the complete consumption of compound **1**. Then compound **2** (0.625 mmol), [RuCl₂(*p*-cym)]₂ (0.025 mmol, 5 mol%), AgSbF₆ (0.25 mmol, 0.5 equiv), Cu(OAc)₂ (1.0 mmol, 2.0 equiv) and 2 mL DCE was added. The reaction system was stirred at 120 °C for 24 h. Then the solvent was removed under reduced pressure. The residue was purified by silica gel column chromatography to afford product **3**.

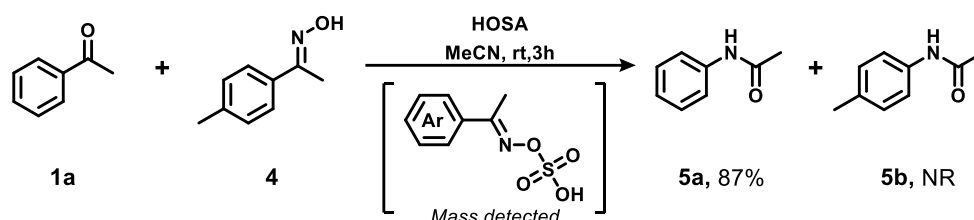
2.3. Competitive Experiment



A reaction tube (10 mL) with magnetic stir bar was charged with compound **1b** (67.1 mg), HOSA (113.1 mg) and 1.0 mL MeCN. Then the mixture was stirred at room temperature for 3h. Another reaction tube (10 mL) with magnetic stir bar was charged with compound **1i** (77.3 mg), HOSA(113.1 mg) and 1.0 mL MeCN. Then the mixture was stirred at room temperature for 3h. TLC (PET: EtOAc= 4:1) showed that the complete consumption of compound **1b** and **1i**. Then compound **2a** (58.1 mg), [RuCl₂(p-cym)]₂ (0.025mmol, 5 mol%), AgSbF₆ (0.25 mmol, 0.5 equiv), Cu(OAc)₂ (1.0 mmol, 2.0 equiv) and 4mL DCE was added, The reaction system was stirred at 120 °C for 24h.

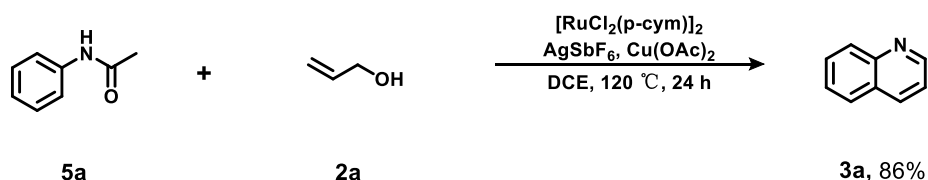
After cooling to room temperature, TLC (PET: EtOAc= 4:1) showed that the reaction was complete. Then the solvent was removed under reduced pressure. The residue was purified by silica gel column chromatography to afford **3b** as yellow oil 58.0 mg and **3j** as yellow oil 15.5 mg.

2.4. Rrearrangement reactions



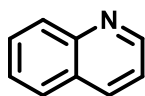
A reaction tube (10 mL) with magnetic stir bar was charged with compound **1a** (60.1 mg), **4** (74.6 mg), HOSA(113.1 mg) and 2.0 mL MeCN. Then the mixture was stirred at room temperature for 3h. TLC (PET: EtOAc= 4:1) showed that the reaction was complete. Then the solvent was removed under reduced pressure. The residue was purified by silica gel column chromatography to afford **5a** as white solids (58.8 mg). **N-phenylacetamide(5a)**: ¹H NMR (400 MHz, CDCl₃) δ 7.75 (s, 1H), 7.50 (d, *J* = 8.1 Hz, 2H), 7.30 (t, *J* = 7.7 Hz, 2H), 7.09 (t, *J* = 7.4 Hz, 1H), 2.15 (s, 3H). ¹³C NMR (101 MHz, CDCl₃) δ 168.83, 138.05, 129.05, 124.41, 120.12, 24.61. HRMS (ESI) *m/z* calcd for C₈H₁₀NO [M+H]⁺ 136.0757, found 136.0758.

2.5. Synthesis of 3a with 5a

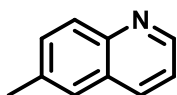


A reaction tube (10 mL) with magnetic stir bar was charged with compound **5a** (0.5 mmol, 1.0 equiv), compound **2a** (43.6mg), [RuCl₂(p-cym)]₂ (0.025mmol, 5 mol%), AgSbF₆ (0.25 mmol, 0.5 equiv), Cu(OAc)₂ (1.0 mmol, 2.0 equiv) and 2 mL DCE was added, The reaction system was stirred at 120 °C for 24h. After cooling to room temperature, TLC (PE: EA= 4:1) showed that the reaction was complete. Then the solvent was removed under reduced pressure. The residue was purified by silica gel column chromatography to afford product **3a** as yellow oil (88.8 mg) in 86 % yield.

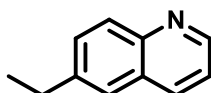
3. Experimental data for described substances



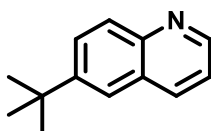
quinoline(3a): The title compound was obtained by column chromatography (PE:EA = 20:1) as yellow oil (54.9 mg) in 85 % yield according to the Method A. ^1H NMR (400 MHz, CDCl_3) δ 8.88 (d, J = 4.1 Hz, 1H), 8.10 (d, J = 8.6 Hz, 2H), 7.77 (d, J = 8.2 Hz, 1H), 7.68 (t, J = 7.7 Hz, 1H), 7.51 (t, J = 7.5 Hz, 1H), 7.36-7.33 (m, 1H). ^{13}C NMR (101 MHz, CDCl_3) δ 150.39, 148.23, 136.15, 129.52, 129.40, 128.31, 127.83, 126.59, 121.11. HRMS (ESI) m/z calcd for $\text{C}_9\text{H}_8\text{N}$ $[\text{M}+\text{H}]^+$ 130.0651, found 130.0652.



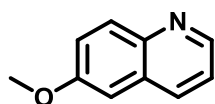
6-methylquinoline(3b): The title compound was obtained by column chromatography (PE:EA = 20:1) as yellow oil (57.3 mg) in 80 % yield according to the Method A. ^1H NMR (400 MHz, CDCl_3) δ 8.82 (d, J = 4.1 Hz, 1H), 8.02-7.97 (m, 2H), 7.52 (d, J = 9.7 Hz, 2H), 7.34-7.30 (m, 1H), 2.51 (s, 3H). ^{13}C NMR (101 MHz, CDCl_3) δ 149.57, 146.92, 136.45, 135.45, 131.82, 129.13, 128.37, 126.65, 121.13, 21.64. HRMS (ESI) m/z calcd for $\text{C}_{10}\text{H}_{10}\text{N}$ $[\text{M}+\text{H}]^+$ 144.0808, found 144.0807.



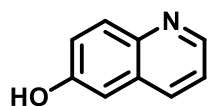
6-ethylquinoline(3c): The title compound was obtained by column chromatography (PE:EA = 20:1) as yellow oil (62.9 mg) in 80 % yield according to the Method A. ^1H NMR (400 MHz, CDCl_3) δ 8.85 – 8.80 (m, 1H), 8.07 – 7.98 (m, 2H), 7.55 (d, J = 7.4 Hz, 2H), 7.33-7.30 (m, 1H), 2.83-2.77 (m, 2H), 1.31 (t, J = 7.6 Hz, 3H). ^{13}C NMR (101 MHz, CDCl_3) δ 149.59, 147.12, 142.63, 135.60, 130.76, 129.26, 128.40, 125.31, 121.07, 28.89, 15.42. HRMS (ESI) m/z calcd for $\text{C}_{11}\text{H}_{12}\text{N}$ $[\text{M}+\text{H}]^+$ 158.0964, found 158.0963.



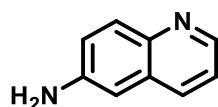
6-(tert-butyl)quinoline(3d): The title compound was obtained by column chromatography (PE:EA = 20:1) as yellow oil (75.0 mg) in 81 % yield according to the Method A. ^1H NMR (400 MHz, CDCl_3) δ 8.84 (d, J = 4.2 Hz, 1H), 8.10 (d, J = 8.3 Hz, 1H), 8.05 (d, J = 8.9 Hz, 1H), 7.80 (d, J = 8.9 Hz, 1H), 7.71 (s, 1H), 7.36-7.33 (m, 1H), 1.41 (s, 9H). ^{13}C NMR (101 MHz, CDCl_3) δ 149.80, 149.45, 146.88, 136.16, 128.98, 128.56, 128.08, 122.78, 121.08, 35.00, 31.27. HRMS (ESI) m/z calcd for $\text{C}_{13}\text{H}_{16}\text{N}$ $[\text{M}+\text{H}]^+$ 186.1277, found 186.1275.



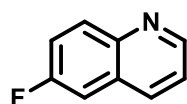
6-methoxyquinoline(3e): The title compound was obtained by column chromatography (PE:EA = 20:1) as yellow oil (62.9 mg) in 79 % yield according to the Method A. ^1H NMR (400 MHz, CDCl_3) δ 8.76 – 8.69 (m, 1H), 8.00–7.96 (m, 2H), 7.37 – 7.27 (m, 2H), 7.01 (s, 1H), 3.88 (s, 3H). ^{13}C NMR (101 MHz, CDCl_3) δ 157.74, 147.93, 144.41, 134.85, 130.83, 129.33, 122.34, 121.40, 105.12, 55.54. HRMS (ESI) m/z calcd for $\text{C}_{10}\text{H}_{10}\text{NO}$ $[\text{M}+\text{H}]^+$ 160.0757, found 160.0756.



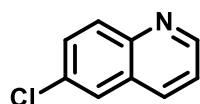
quinolin-6-ol(3f): The title compound was obtained by column chromatography (PE:EA = 10:1) as yellow oil (14.5 mg) in 20 % yield according to the Method A. ^1H NMR (400 MHz, DMSO) δ 9.87 (s, 1H), 8.49 – 8.36 (m, 1H), 7.89 (d, J = 8.3 Hz, 1H), 7.66 (d, J = 9.1 Hz, 1H), 7.16 – 7.09 (m, 2H), 6.94 (s, 1H). ^{13}C NMR (101 MHz, DMSO) δ 155.57, 147.16, 143.11, 134.20, 130.47, 129.40, 122.08, 121.44, 108.4. HRMS (ESI) m/z calcd for $\text{C}_9\text{H}_8\text{NO}$ $[\text{M}+\text{H}]^+$ 146.06, found 146.0589.



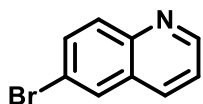
quinolin-6-amine(3g): The title compound was obtained by column chromatography (PE:EA = 10:1) as yellow solids (13.6 mg) in 19 % yield according to the Method A. ^1H NMR (400 MHz, CDCl_3) δ 8.62 (d, J = 4.0 Hz, 1H), 7.90–7.82 (m, 2H), 7.24–7.21 (m, 1H), 7.12–7.09 (m, 1H), 6.84 (s, 1H), 3.94 (s, 2H). ^{13}C NMR (101 MHz, CDCl_3) δ 146.77, 144.78, 143.39, 133.82, 130.48, 129.82, 121.64, 121.42, 107.39. HRMS (ESI) m/z calcd for $\text{C}_9\text{H}_9\text{N}_2$ $[\text{M}+\text{H}]^+$ 145.076, found 145.0758.



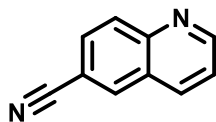
6-fluoroquinoline(3h): The title compound was obtained by column chromatography (PE:EA = 20:1) as yellow oil (43.4 mg) in 59 % yield according to the Method A. ^1H NMR (400 MHz, CDCl_3) δ 8.84 (d, J = 4.1 Hz, 1H), 8.10 – 8.04 (m, 2H), 7.47–7.44 (m, 1H), 7.40 – 7.34 (m, 2H). ^{13}C NMR (101 MHz, $\text{Chloroform-}d$) δ 73.32, 73.54, 82.37, 82.63, 84.50, 91.55, 91.65, 94.60, 94.69, 98.17, 98.22, 108.04, 112.36, 112.39, 121.86, 124.33. HRMS (ESI) m/z calcd for $\text{C}_9\text{H}_7\text{FN}$ $[\text{M}+\text{H}]^+$ 148.0557, found 148.0555.



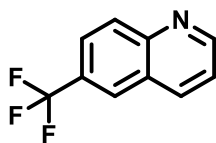
6-chloroquinoline(3i): The title compound was obtained by column chromatography (PE:EA =20:1) as yellow oil (49.9 mg) in 61 % yield according to the Method A. ^1H NMR (400 MHz, CDCl_3) δ 8.86 (d, J = 3.9 Hz, 1H), 8.00 (d, J = 8.7 Hz, 2H), 7.73 (d, J = 1.4 Hz, 1H), 7.61-7.58 (m, 1H), 7.38-7.34 (m, 1H). ^{13}C NMR (101 MHz, CDCl_3) δ 150.64, 146.65, 135.16, 132.31, 131.14, 130.44, 128.85, 126.46, 121.95. HRMS (ESI) m/z calcd for $\text{C}_9\text{H}_7^{35.5}\text{ClN}$ $[\text{M}+\text{H}]^+$ 164.0262, found 164.0262.



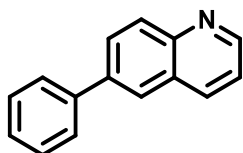
6-bromoquinoline(3j): The title compound was obtained by column chromatography (PE:EA = 20:1) as yellow oil (57.2 mg) in 55 % yield according to the Method A. ^1H NMR (400 MHz, CDCl_3) δ 8.90 – 8.84 (m, 1H), 7.99 (d, J = 8.3 Hz, 1H), 7.95 – 7.89 (m, 2H), 7.72 (d, J = 9.0 Hz, 1H), 7.37-7.34 (m, 1H). ^{13}C NMR (101 MHz, CDCl_3) δ 150.75, 146.81, 135.07, 132.96, 131.22, 129.82, 129.34, 121.91, 120.48. HRMS (ESI) m/z calcd for $\text{C}_9\text{H}_7^{79}\text{BrN}$ $[\text{M}+\text{H}]^+$ 207.9756, found 207.9755.



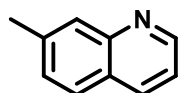
quinoline-6-carbonitrile(3k): The title compound was obtained by column chromatography (PE:EA = 20:1) as yellow oil (50.9 mg) in 66 % yield according to the Method A. ^1H NMR (400 MHz, CDCl_3) δ 9.08 (s, 1H), 8.22-8.15 (m, 3H), 7.82 (d, J = 8.3 Hz, 1H), 7.53 (d, J = 4.7 Hz, 1H). ^{13}C NMR (101 MHz, CDCl_3) δ 153.18, 149.22, 136.41, 134.22, 131.14, 130.15, 127.74, 122.93, 118.54, 110.41. HRMS (ESI) m/z calcd for $\text{C}_{10}\text{H}_7\text{N}_2$ $[\text{M}+\text{H}]^+$ 155.0604, found 155.0605.



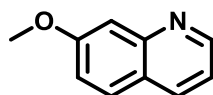
6-(trifluoromethyl)quinoline(3l): The title compound was obtained by column chromatography (PE:EA = 20:1) as yellow oil (57.2 mg) in 58 % yield according to the Method A. ^1H NMR (400 MHz, CDCl_3) δ 9.07 – 9.00 (m, 1H), 8.28 – 8.19 (m, 2H), 8.14 (s, 1H), 7.89 (d, J = 8.8 Hz, 1H), 7.53-7.49 (m, 1H). ^{13}C NMR (101 MHz, CDCl_3) δ 152.62 (s), 149.28 (s), 137.02 (s), 130.85 (s), 128.62 (q, J = 32.3 Hz), 127.34 (s), 125.94 (q, J = 4.3 Hz), 125.30 (q, J = 2.9 Hz), 124.09 (q, J = 270.5 Hz), 122.41 (s). HRMS (ESI) m/z calcd for $\text{C}_{10}\text{H}_7\text{F}_3\text{N}$ $[\text{M}+\text{H}]^+$ 198.0531, found 198.0533.



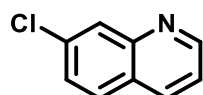
6-phenylquinoline(3m): The title compound was obtained by column chromatography (PE:EA = 20:1) as yellow oil (72.9 mg) in 71 % yield according to the Method A. ¹H NMR (400 MHz, CDCl₃) δ 8.22-8.17 (m, 4H), 7.87 (d, *J* = 8.6 Hz, 1H), 7.83 (d, *J* = 8.1 Hz, 1H), 7.74 (t, *J* = 7.6 Hz, 1H), 7.59 – 7.44 (m, 4H). ¹³C NMR (101 MHz, CDCl₃) δ 157.46, 148.37, 139.77, 136.89, 129.82, 129.77, 129.43, 128.95, 127.68, 127.57, 127.28, 126.38, 119.11. HRMS (ESI) *m/z* calcd for C₁₅H₁₂N [M+H]⁺ 206.0964, found 206.0971.



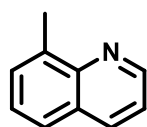
7-methylquinoline(3n): The title compound was obtained by column chromatography (PE:EA = 20:1) as yellow oil (47.3 mg) in 66 % yield according to the Method A. ¹H NMR (400 MHz, CDCl₃) δ 8.85 (d, *J* = 4.0 Hz, 1H), 8.07 (d, *J* = 8.2 Hz, 1H), 7.87 (s, 1H), 7.67 (d, *J* = 8.3 Hz, 1H), 7.35 (d, *J* = 8.3 Hz, 1H), 7.31-7.27 (m, 1H), 2.54 (s, 3H). ¹³C NMR (101 MHz, CDCl₃) δ 150.41, 148.54, 139.80, 135.78, 128.86, 128.45, 127.48, 126.39, 120.34, 21.96. HRMS (ESI) *m/z* calcd for C₁₀H₁₀N [M+H]⁺ 144.0808, found 144.0808.



7-methoxyquinoline(3o): The title compound was obtained by column chromatography (PE:EA = 20:1) as yellow oil (48.6 mg) in 61 % yield according to the Method A. ¹H NMR (400 MHz, CDCl₃) δ 8.79 (s, 1H), 8.01 (d, *J* = 7.7 Hz, 1H), 7.63 (d, *J* = 8.8 Hz, 1H), 7.39 (s, 1H), 7.23 – 7.13 (m, 2H), 3.90 (s, 3H). ¹³C NMR (101 MHz, CDCl₃) δ 160.67, 150.56, 149.96, 135.70, 128.82, 123.54, 119.82, 119.00, 107.29, 55.50. HRMS (ESI) *m/z* calcd for C₁₀H₁₀NO [M+H]⁺ 160.0757, found 160.0756.

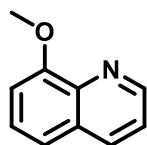


7-chloroquinoline(3p): The title compound was obtained by column chromatography (PE:EA = 20:1) as yellow oil (49.1 mg) in 60 % yield according to the Method A. ¹H NMR (400 MHz, CDCl₃) δ 8.89 (d, *J* = 4.1 Hz, 1H), 8.10 (d, *J* = 12.3 Hz, 2H), 7.72 (d, *J* = 8.7 Hz, 1H), 7.47 (d, *J* = 8.7 Hz, 1H), 7.39-7.36 (m, 1H). ¹³C NMR (101 MHz, CDCl₃) δ 151.39, 148.56, 136.03, 135.40, 129.13, 128.47, 127.76, 126.69, 121.35. HRMS (ESI) *m/z* calcd for C₉H₇^{35,37}ClN [M+H]⁺ 164.0262, found 164.0263.

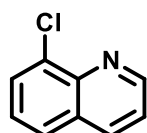


8-methylquinoline(3q): The title compound was obtained by column chromatography (PE:EA = 20:1) as yellow oil (53.0 mg) in 74 % yield according to the Method A. ¹H NMR (400 MHz, CDCl₃) δ 8.97 – 8.92 (m, 1H), 8.11 (d, *J* = 8.2 Hz, 1H), 7.65 (d, *J* = 8.1 Hz, 1H), 7.56 (d, *J* = 6.9 Hz, 1H), 7.46 – 7.34 (m, 2H),

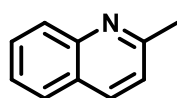
2.83 (s, 3H). ^{13}C NMR (101 MHz, CDCl_3) δ 149.34, 147.44, 137.15, 136.42, 129.72, 128.35, 126.39, 125.97, 120.93, 18.28. HRMS (ESI) m/z calcd for $\text{C}_{10}\text{H}_{10}\text{N}$ $[\text{M}+\text{H}]^+$ 144.0808, found 144.0809.



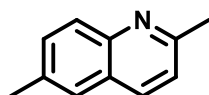
8-methoxyquinoline(3r): The title compound was obtained by column chromatography (PE:EA = 20:1) as yellow oil (39.1 mg) in 49 % yield according to the Method A. ^1H NMR (400 MHz, CDCl_3) δ 8.86 (d, J = 4.1 Hz, 1H), 8.04 (d, J = 8.3 Hz, 1H), 7.41-7.29 (m, 3H), 6.98 (d, J = 7.6 Hz, 1H), 4.02 (s, 3H). ^{13}C NMR (101 MHz, CDCl_3) δ 155.30, 149.17, 140.11, 135.85, 129.28, 126.67, 121.64, 119.50, 107.49, 55.91. HRMS (ESI) m/z calcd for $\text{C}_{10}\text{H}_{10}\text{NO}$ $[\text{M}+\text{H}]^+$ 160.0757, found 160.0754.



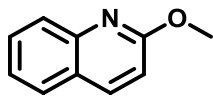
8-chloroquinoline(3s): The title compound was obtained by column chromatography (PE:EA = 20:1) as yellow oil (43.2 mg) in 53 % yield according to the Method A. ^1H NMR (400 MHz, CDCl_3) δ 9.04 – 8.97 (m, 1H), 8.14 (d, J = 8.3 Hz, 1H), 7.80 (d, J = 7.5 Hz, 1H), 7.70 (d, J = 8.2 Hz, 1H), 7.46 – 7.39 (m, 2H). ^{13}C NMR (101 MHz, CDCl_3) δ 151.05, 144.46, 136.61, 133.46, 129.67, 129.62, 127.06, 126.57, 121.99. HRMS (ESI) m/z calcd for $\text{C}_9\text{H}_7^{35,37}\text{ClN}$ $[\text{M}+\text{H}]^+$ 164.0262, found 164.0261.



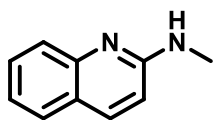
2-methylquinoline(3t): The title compound was obtained by column chromatography (PE:EA = 20:1) as yellow oil (50.1 mg) in 70 % yield according to the Method A. ^1H NMR (400 MHz, CDCl_3) δ 8.04 (dd, J = 8.3, 4.8 Hz, 2H), 7.77 (d, J = 8.1 Hz, 1H), 7.69 (t, J = 7.7 Hz, 1H), 7.49 (t, J = 7.5 Hz, 1H), 7.28 (d, J = 8.4 Hz, 1H), 2.76 (s, 3H). ^{13}C NMR (101 MHz, CDCl_3) δ 159.04, 147.91, 136.22, 129.48, 128.68, 127.55, 126.53, 125.72, 122.05, 25.46. HRMS (ESI) m/z calcd for $\text{C}_{10}\text{H}_{10}\text{N}$ $[\text{M}+\text{H}]^+$ 144.0808, found 144.0810.



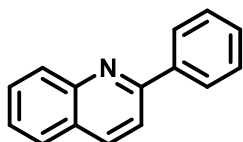
2-ethylquinoline(3u): The title compound was obtained by column chromatography (PE:EA = 20:1) as yellow oil (54.2 mg) in 69 % yield according to the Method A. ^1H NMR (400 MHz, CDCl_3) δ 7.85 (d, J = 8.5 Hz, 1H), 7.77 (d, J = 8.4 Hz, 1H), 7.43 – 7.32 (m, 2H), 7.08 (d, J = 8.4 Hz, 1H), 2.62 (s, 3H), 2.38 (s, 3H). ^{13}C NMR (101 MHz, CDCl_3) δ 157.73, 146.27, 135.32, 135.12, 131.43, 128.14, 126.30, 126.23, 121.74, 25.09, 21.27. HRMS (ESI) m/z calcd for $\text{C}_{11}\text{H}_{12}\text{N}$ $[\text{M}+\text{H}]^+$ 158.0964, found 158.0964.



2-methoxyquinoline(3v): The title compound was obtained by column chromatography (PE:EA = 20:1) as yellow oil (53.3 mg) in 67 % yield according to the Method A. ^1H NMR (400 MHz, CDCl_3) δ 7.96 (d, J = 8.8 Hz, 1H), 7.88 (d, J = 8.4 Hz, 1H), 7.71 (d, J = 8.0 Hz, 1H), 7.63 (t, J = 7.7 Hz, 1H), 7.38 (t, J = 7.5 Hz, 1H), 6.91 (d, J = 8.8 Hz, 1H), 4.10 (s, 3H). ^{13}C NMR (101 MHz, CDCl_3) δ 162.51, 146.69, 138.76, 129.58, 127.54, 127.33, 125.18, 124.08, 113.17, 53.48. HRMS (ESI) m/z calcd for $\text{C}_{10}\text{H}_{10}\text{NO}$ $[\text{M}+\text{H}]^+$ 160.0757, found 160.0726.



N-methylquinolin-2-amine(3w): The title compound was obtained by column chromatography (PE:EA = 20:1) as yellow oil (44.3 mg) in 56 % yield according to the Method A. ^1H NMR (400 MHz, CDCl_3) δ 7.80 (d, J = 8.9 Hz, 1H), 7.71 (d, J = 8.4 Hz, 1H), 7.59 – 7.50 (m, 2H), 7.20 (t, J = 7.4 Hz, 1H), 6.62 (d, J = 8.9 Hz, 1H), 4.89 (s, 1H), 3.07 (d, J = 3.6 Hz, 3H). ^{13}C NMR (101 MHz, CDCl_3) δ 157.77, 148.15, 137.34, 129.64, 127.56, 126.11, 123.42, 122.05, 111.31, 28.78. HRMS (ESI) m/z calcd for $\text{C}_{10}\text{H}_{11}\text{N}_2$ $[\text{M}+\text{H}]^+$ 159.0917, found 159.0919.

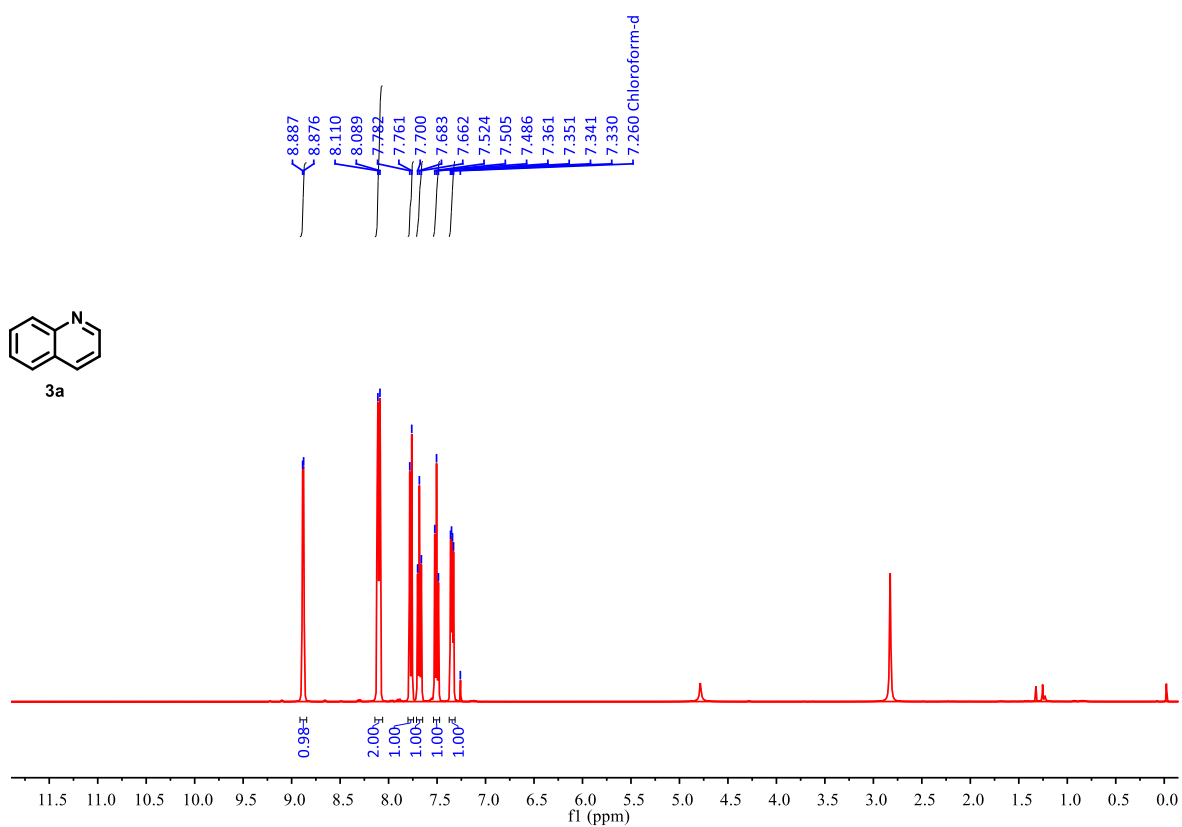


2-phenylquinoline(3x): The title compound was obtained by column chromatography (PE:EA = 20:1) as yellow oil (48.2 mg) in 47 % yield according to the Method A. ^1H NMR (400 MHz, CDCl_3) δ 8.26 – 8.15 (m, 4H), 7.87-7.80 (m, 2H), 7.75 (t, J = 7.7 Hz, 1H), 7.59 – 7.45 (m, 4H). ^{13}C NMR (101 MHz, CDCl_3) δ 157.38, 148.31, 139.71, 136.83, 129.76, 129.72, 129.39, 128.90, 127.64, 127.53, 127.22, 126.33, 119.05. HRMS (ESI) m/z calcd for $\text{C}_{15}\text{H}_{12}\text{N}$ $[\text{M}+\text{H}]^+$ 206.0964, found 206.0976.

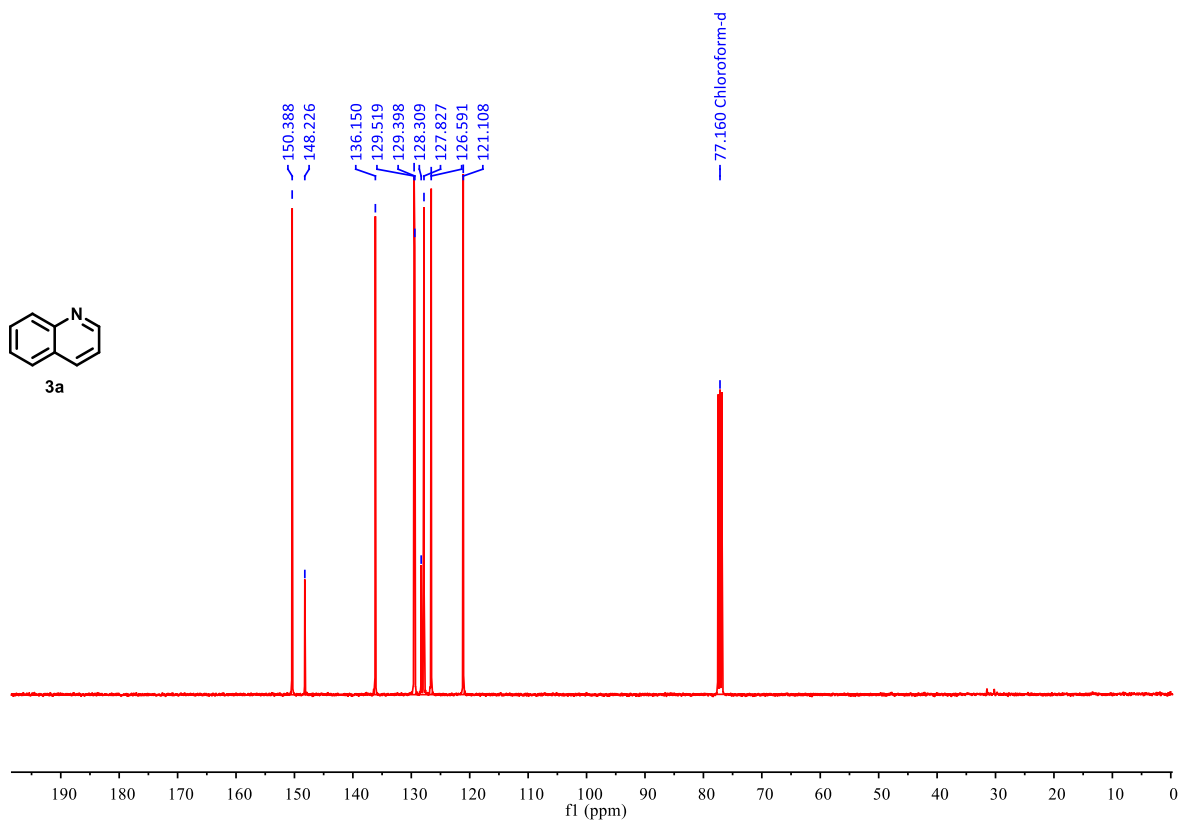
4. Copies of ^1H and ^{13}C NMR

quinoline(5a):

^1H NMR, 400 MHz, CDCl_3

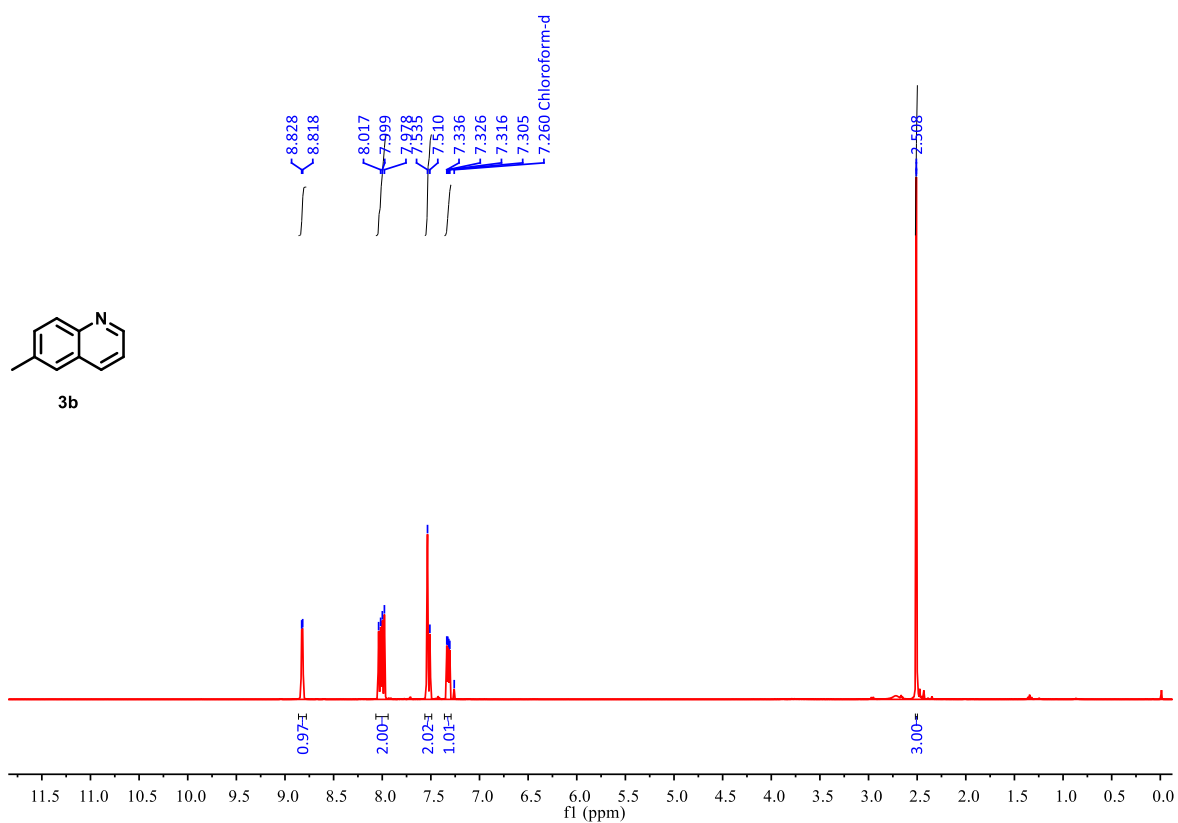


¹³C NMR, 101 MHz, CDCl₃

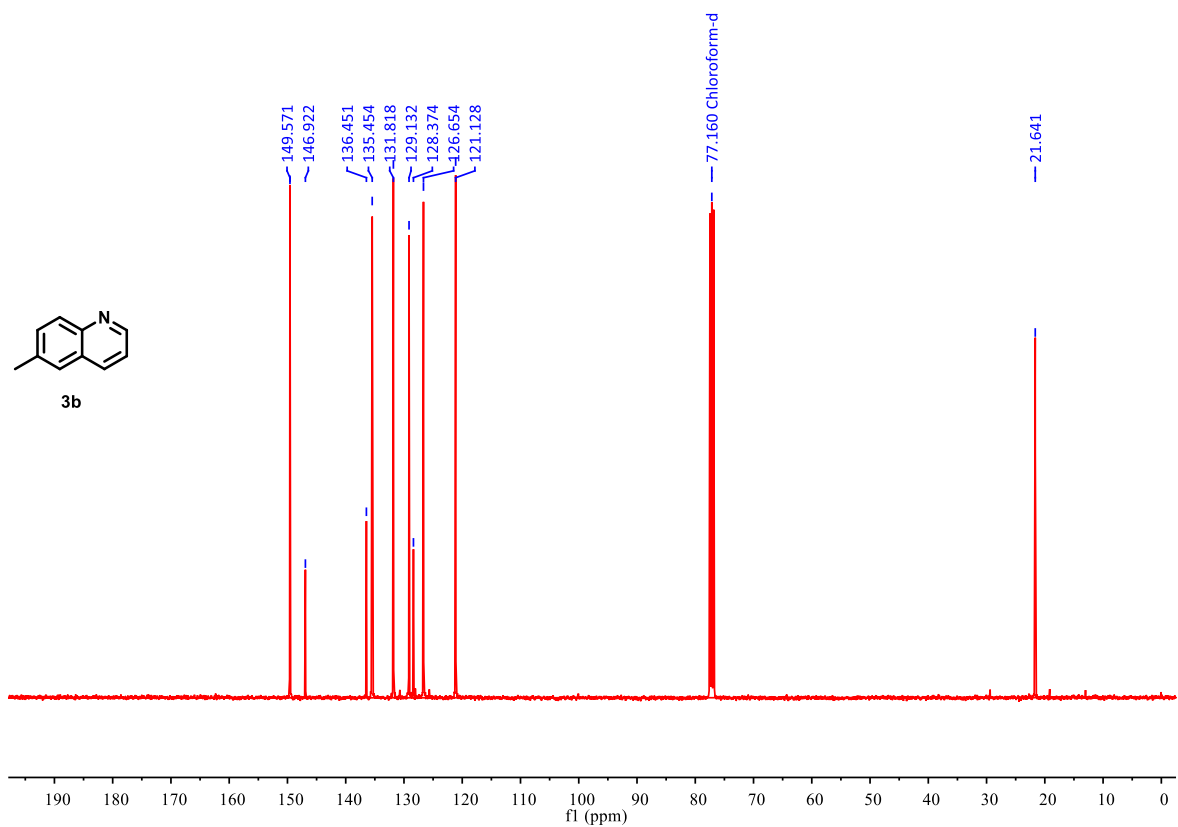


6-methylquinoline(3b):

¹H NMR, 400 MHz, CDCl₃

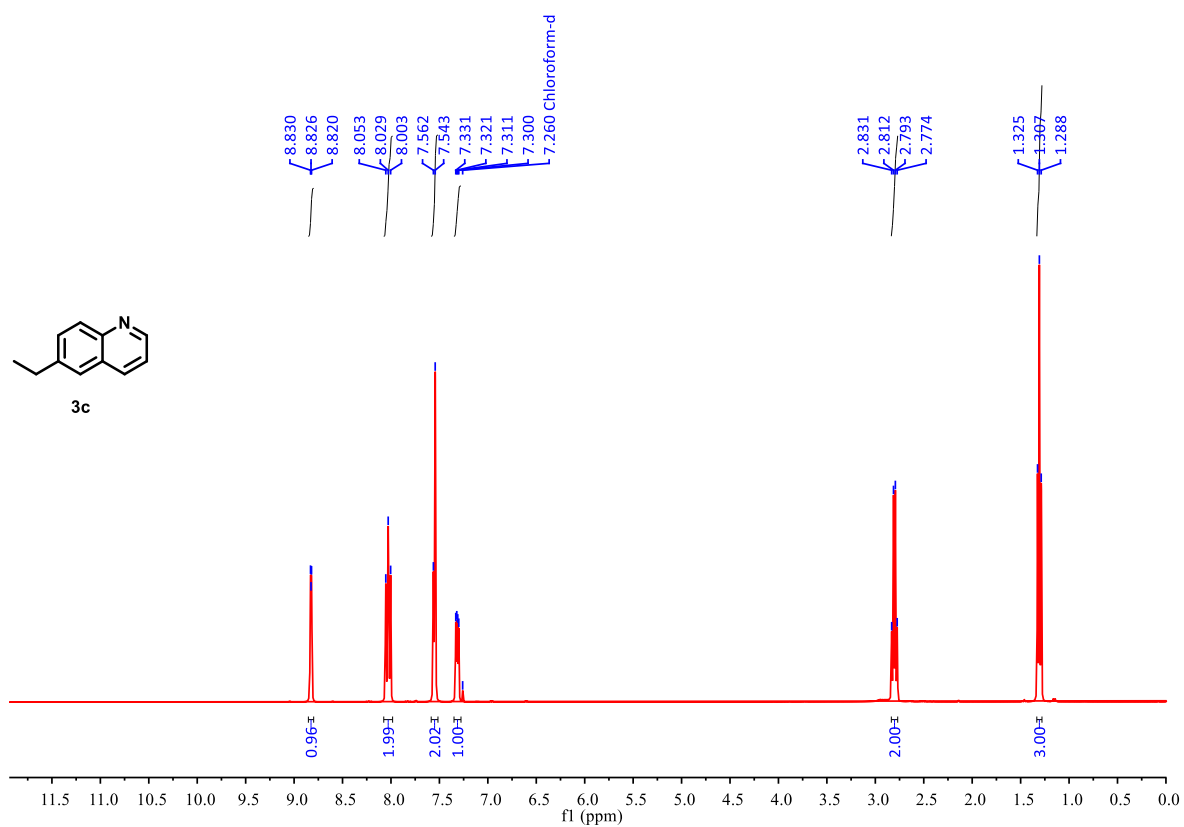


¹³C NMR, 101 MHz, CDCl₃

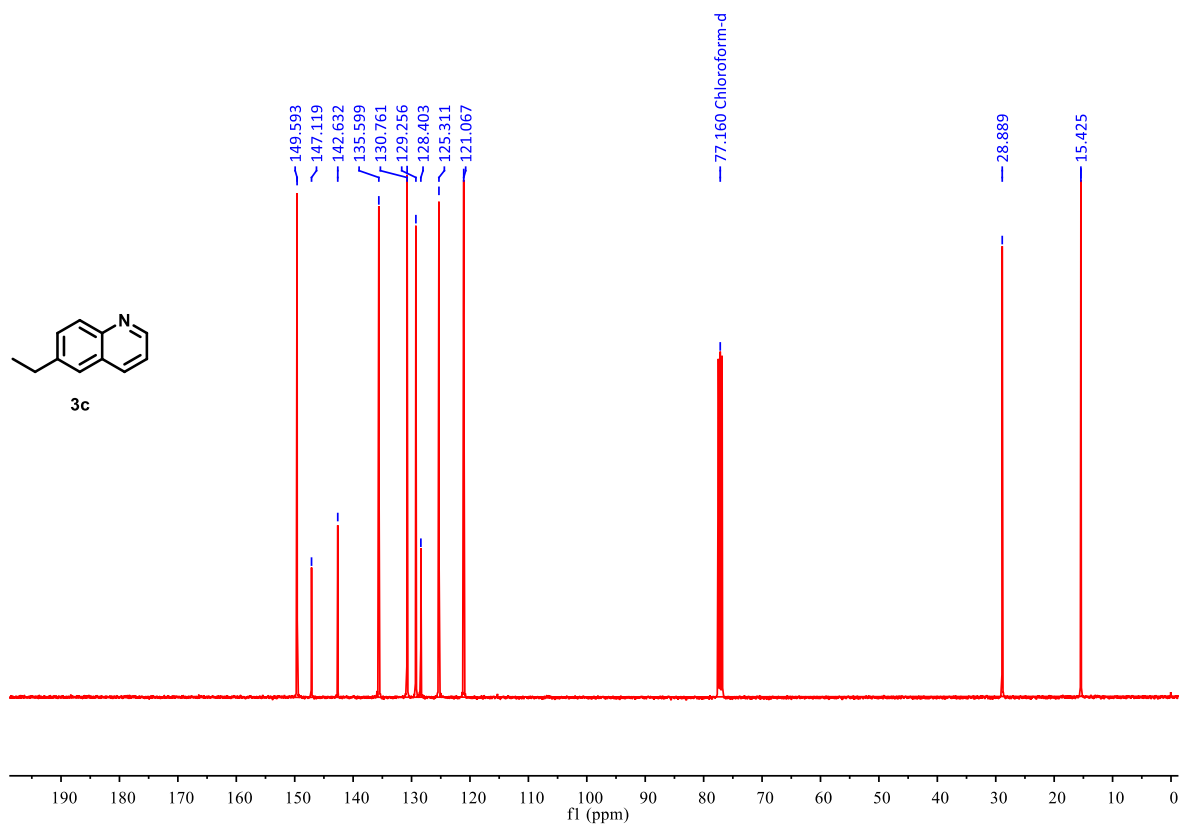


6-ethylquinoline(3c):

¹H NMR, 400 MHz, CDCl₃

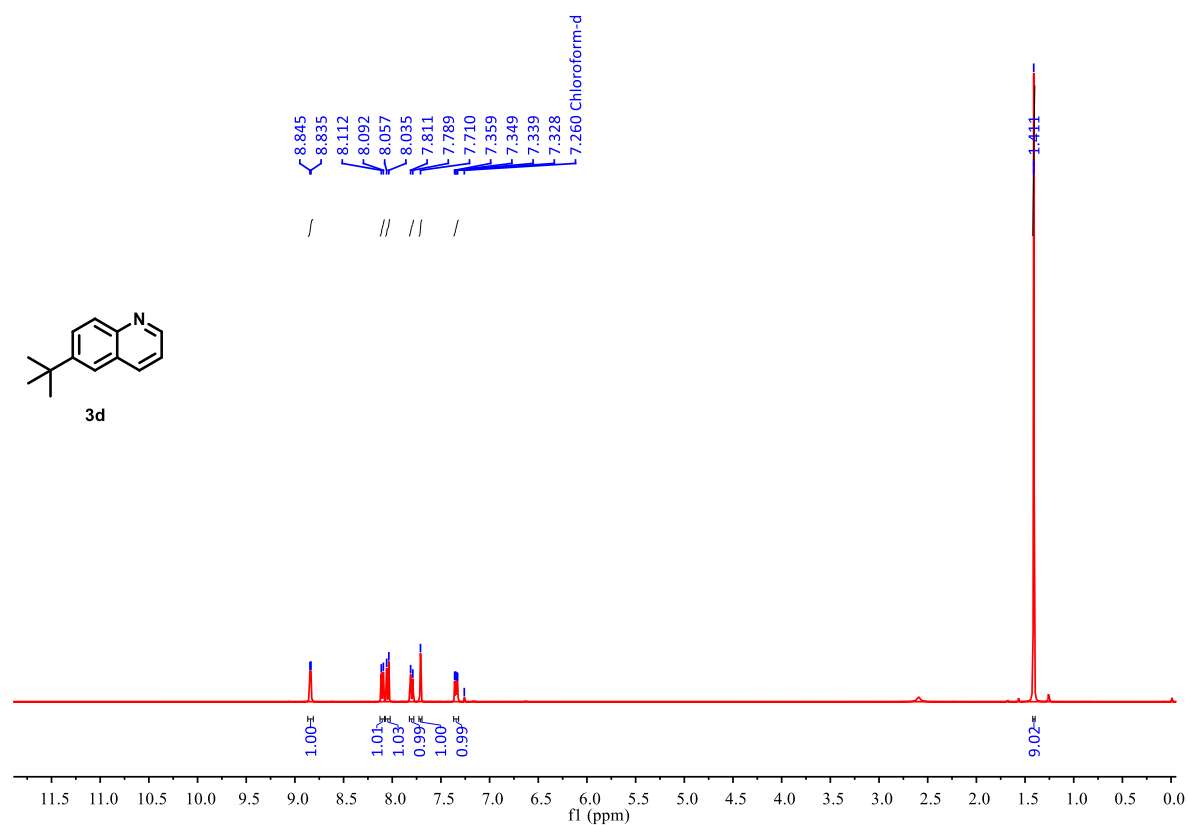


¹³C NMR, 101 MHz, CDCl₃

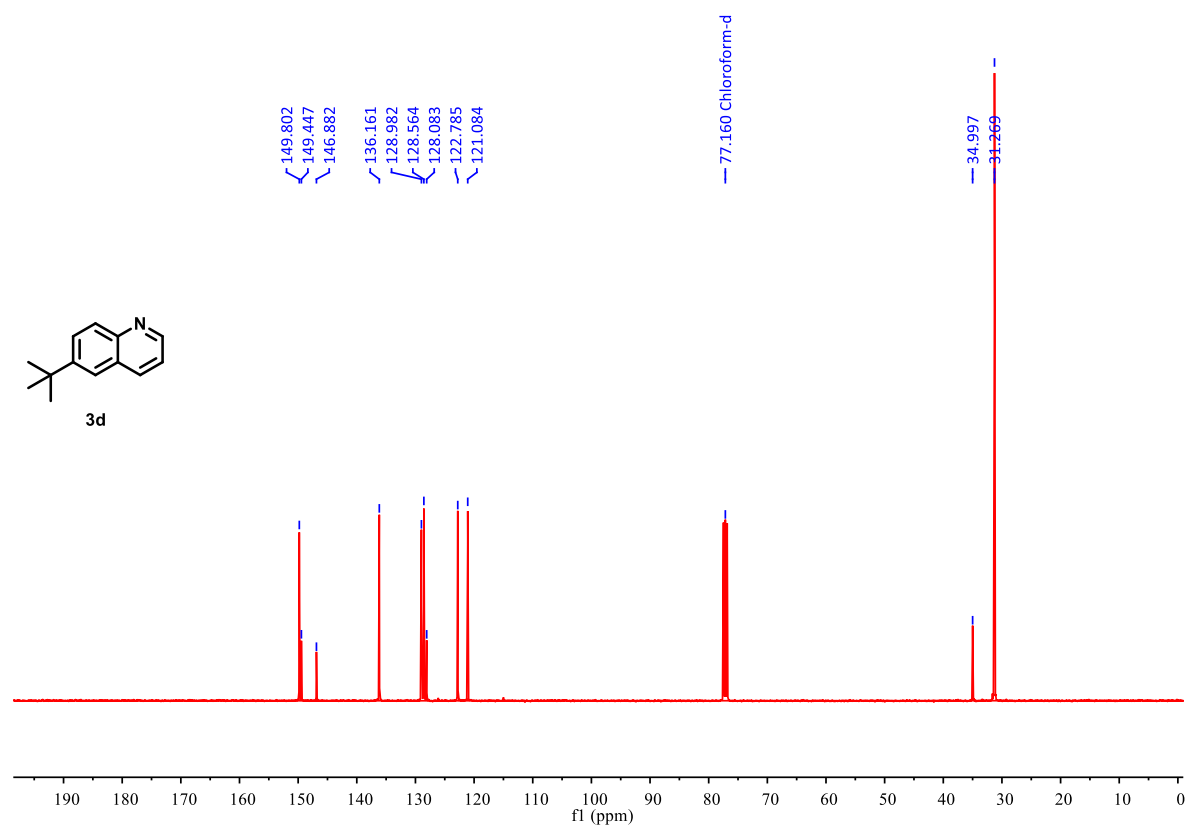


6-(tert-butyl)quinoline(3d):

¹H NMR, 400 MHz, CDCl₃

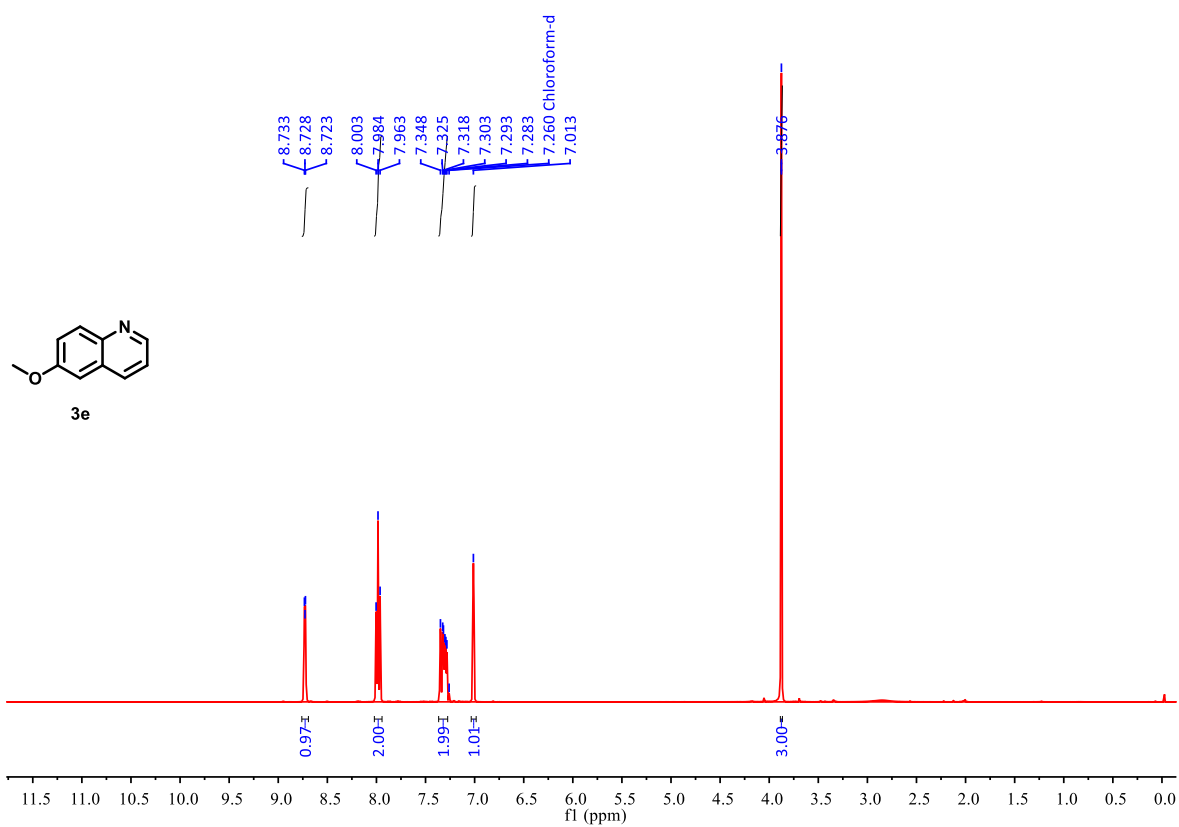


¹³C NMR, 101 MHz, CDCl₃

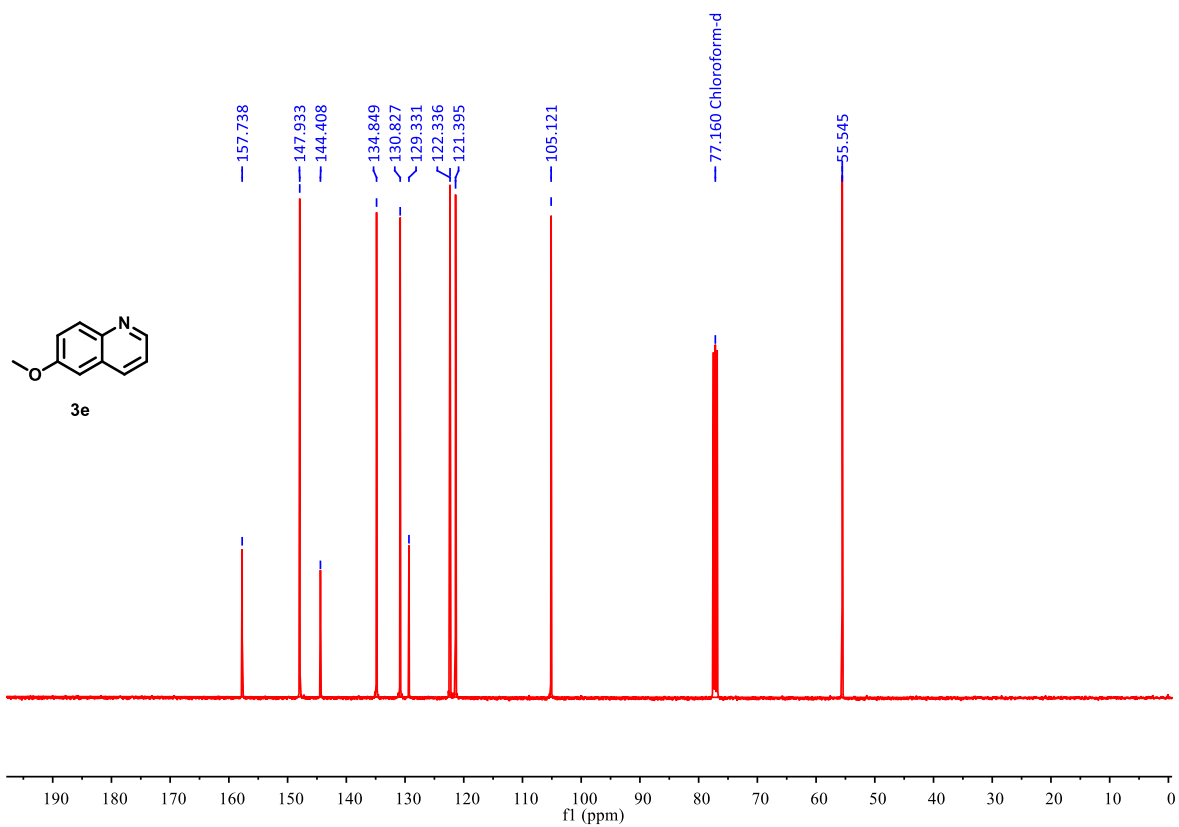


6-methoxyquinoline(3e):

¹H NMR, 400 MHz, CDCl₃

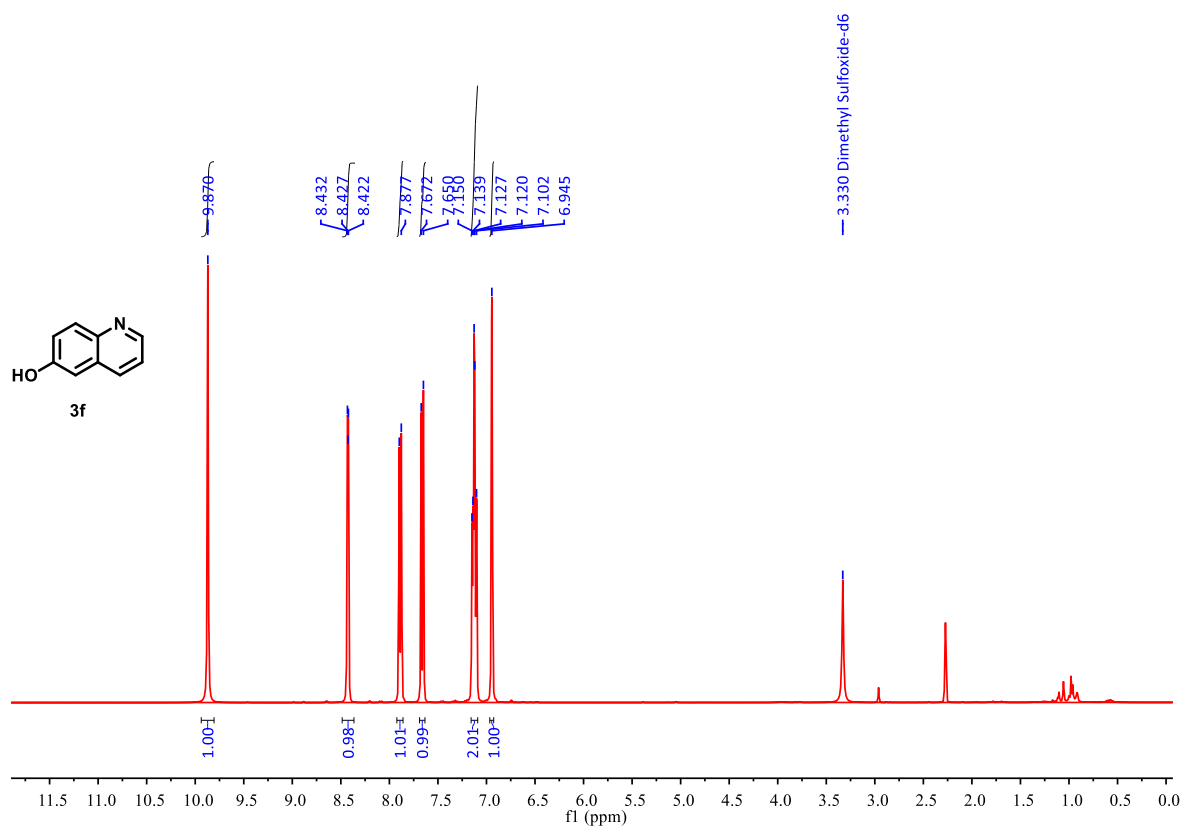


¹³C NMR, 101 MHz, CDCl₃

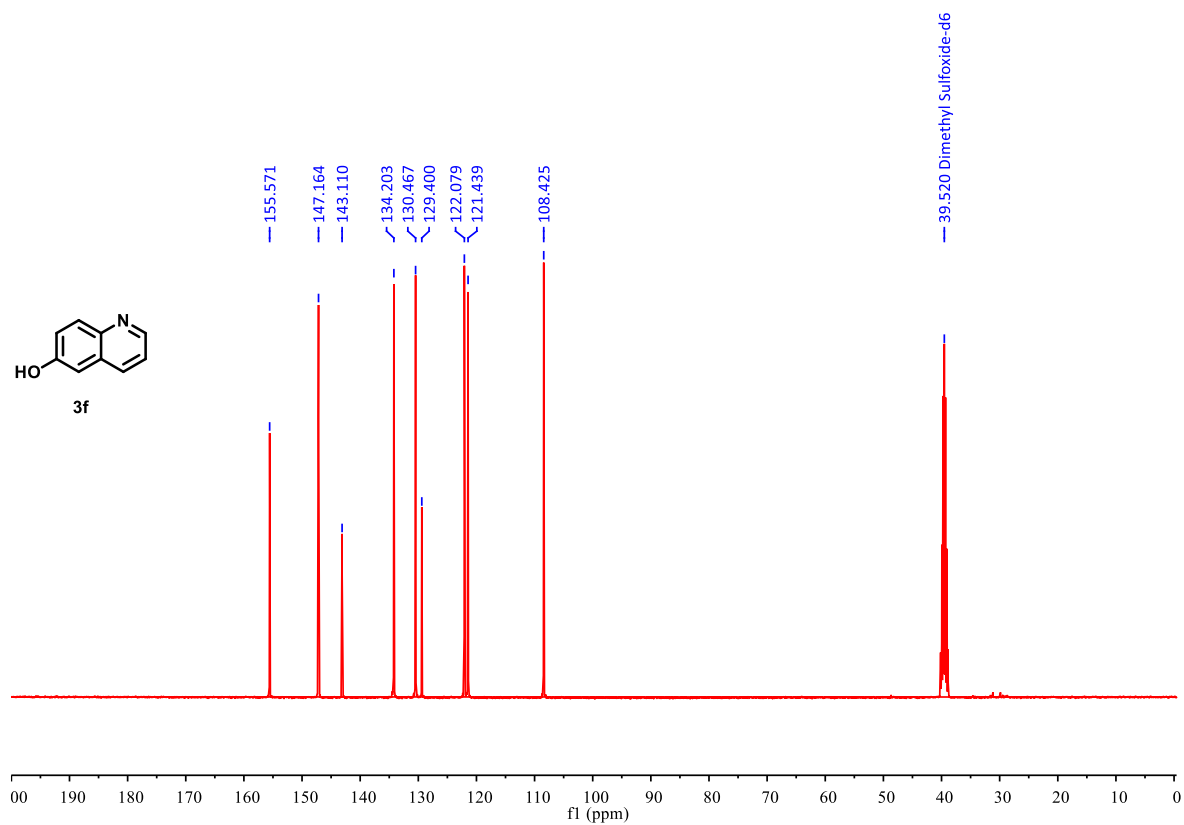


quinolin-6-ol(3f):

¹H NMR, 400 MHz, CDCl₃

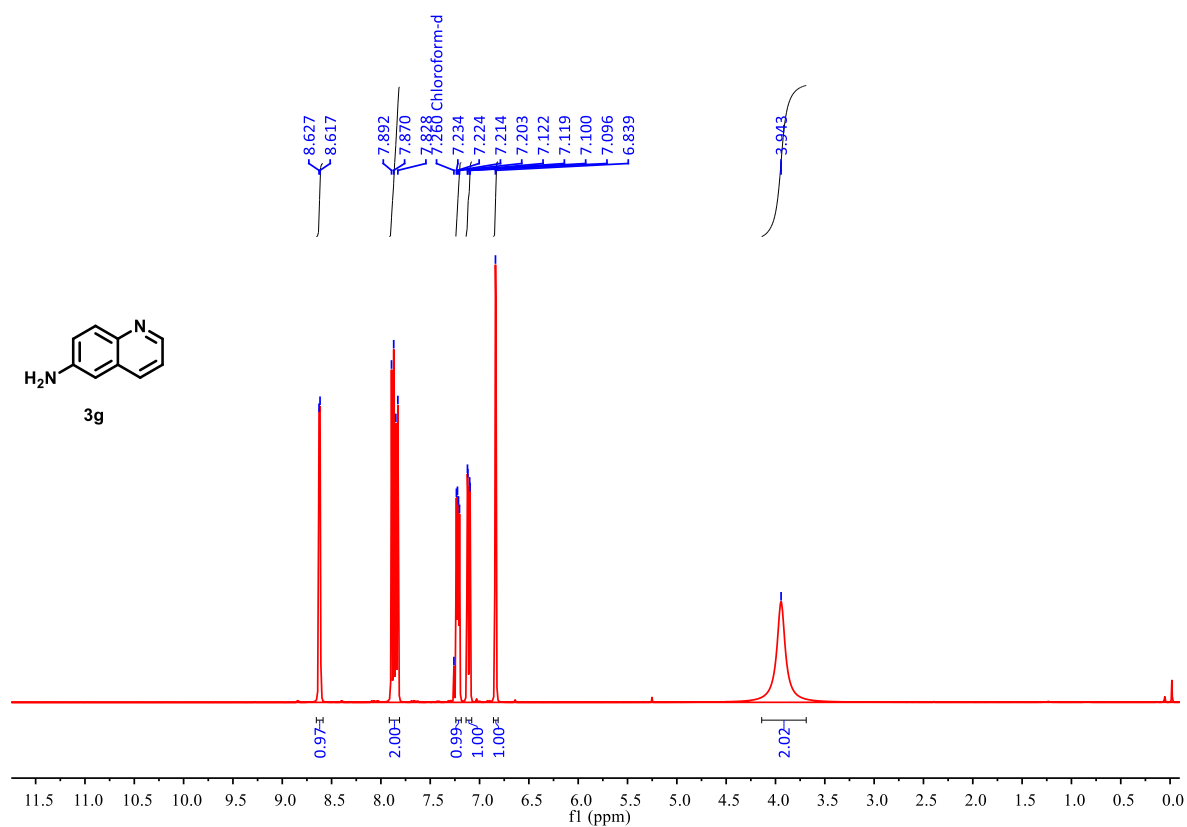


¹³C NMR, 101 MHz, CDCl₃

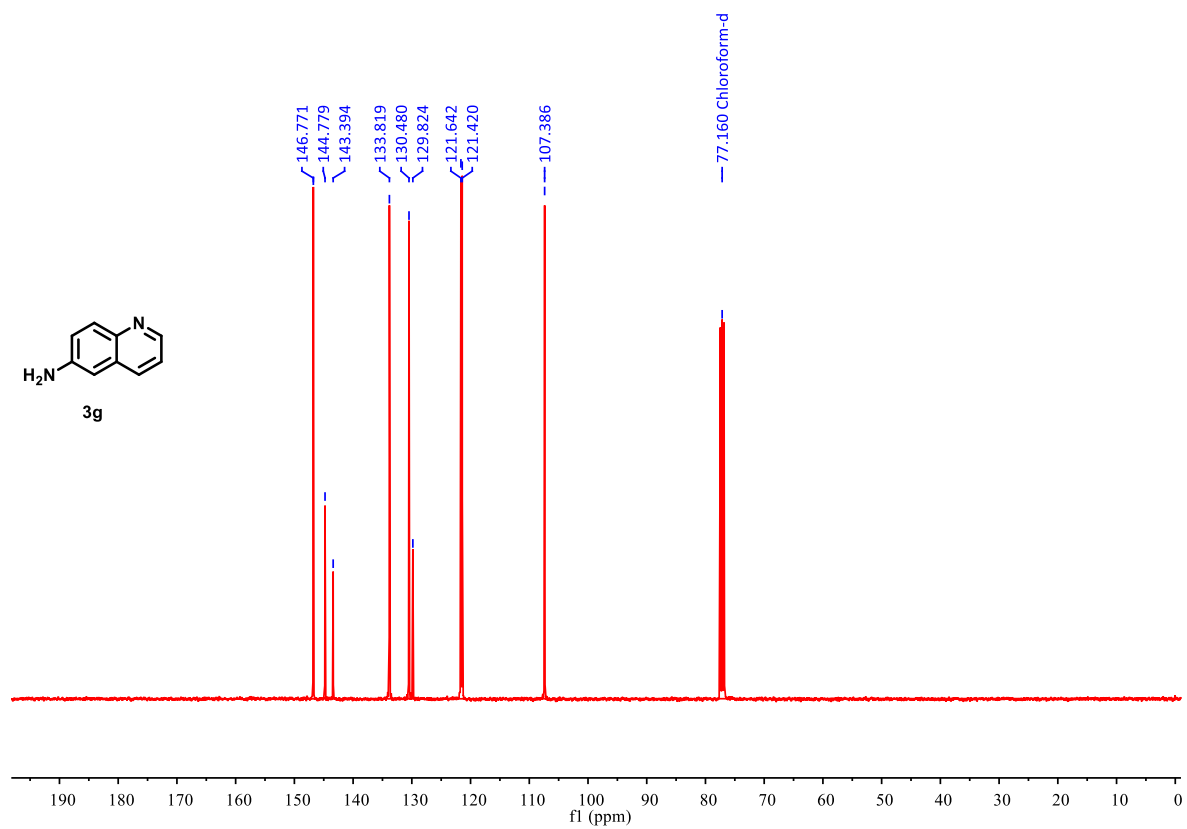


quinolin-6-amine(3g):

¹H NMR, 400 MHz, CDCl₃

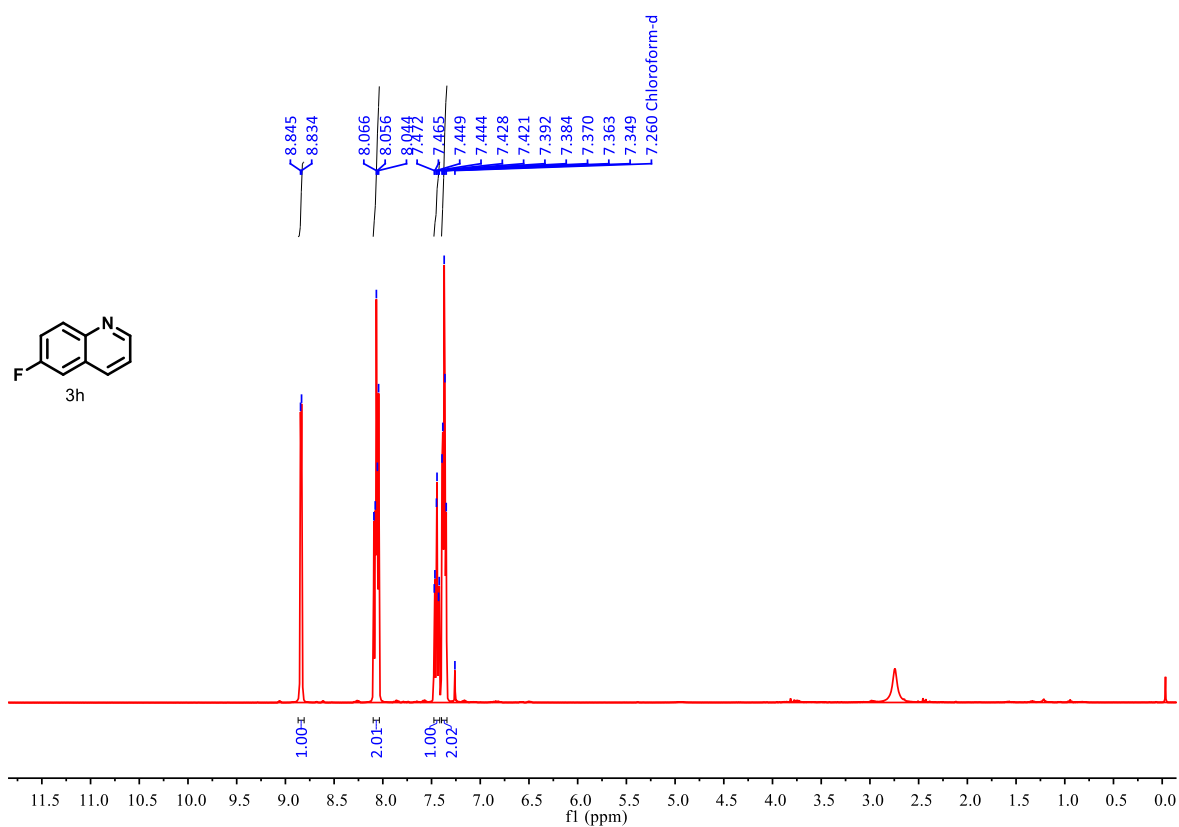


¹³C NMR, 101 MHz, CDCl₃

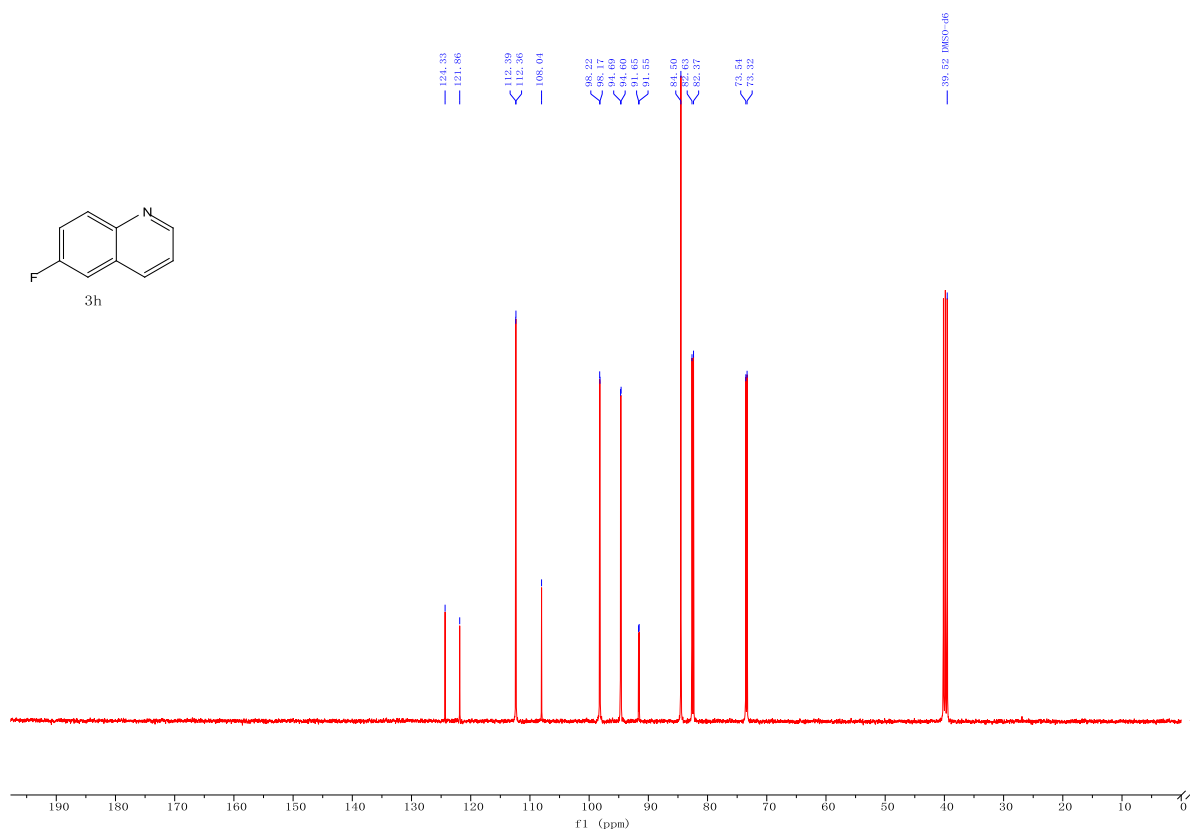


6-fluoroquinoline(3h):

¹H NMR, 400 MHz, CDCl₃

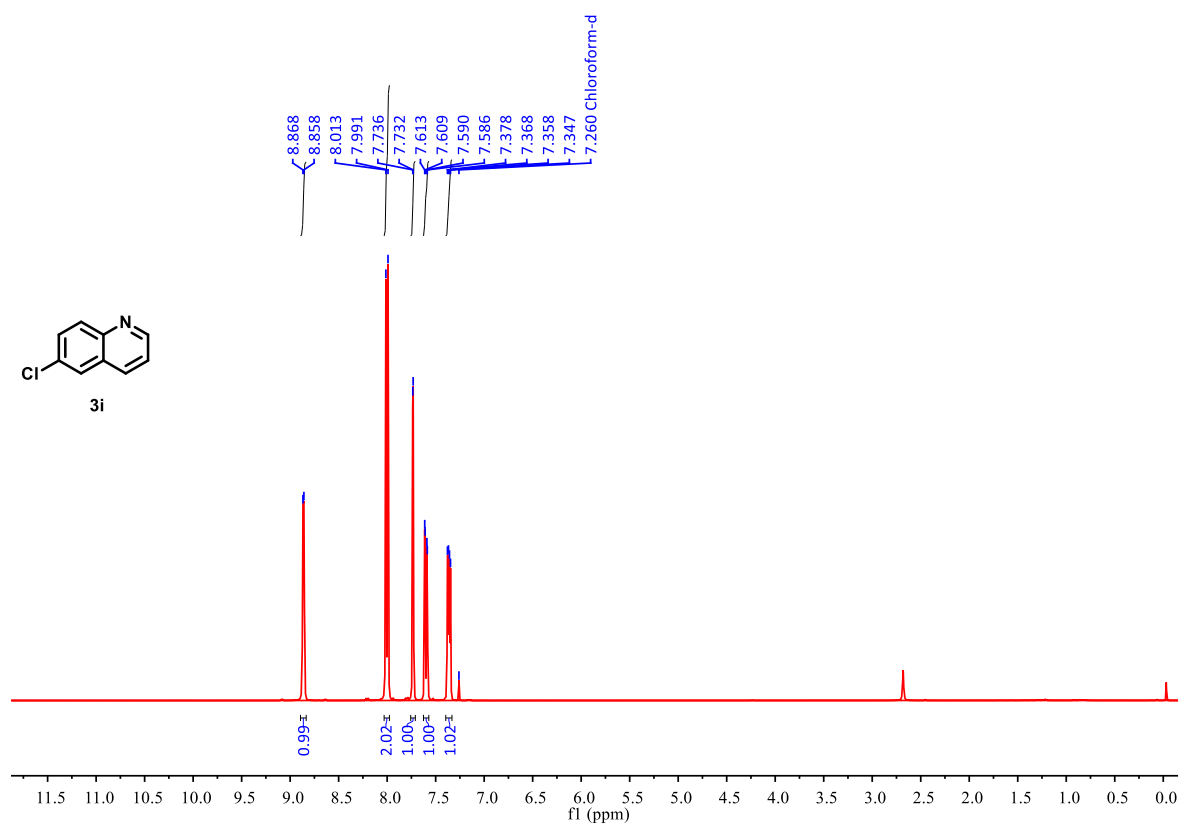


¹³C NMR, 101 MHz, CDCl₃

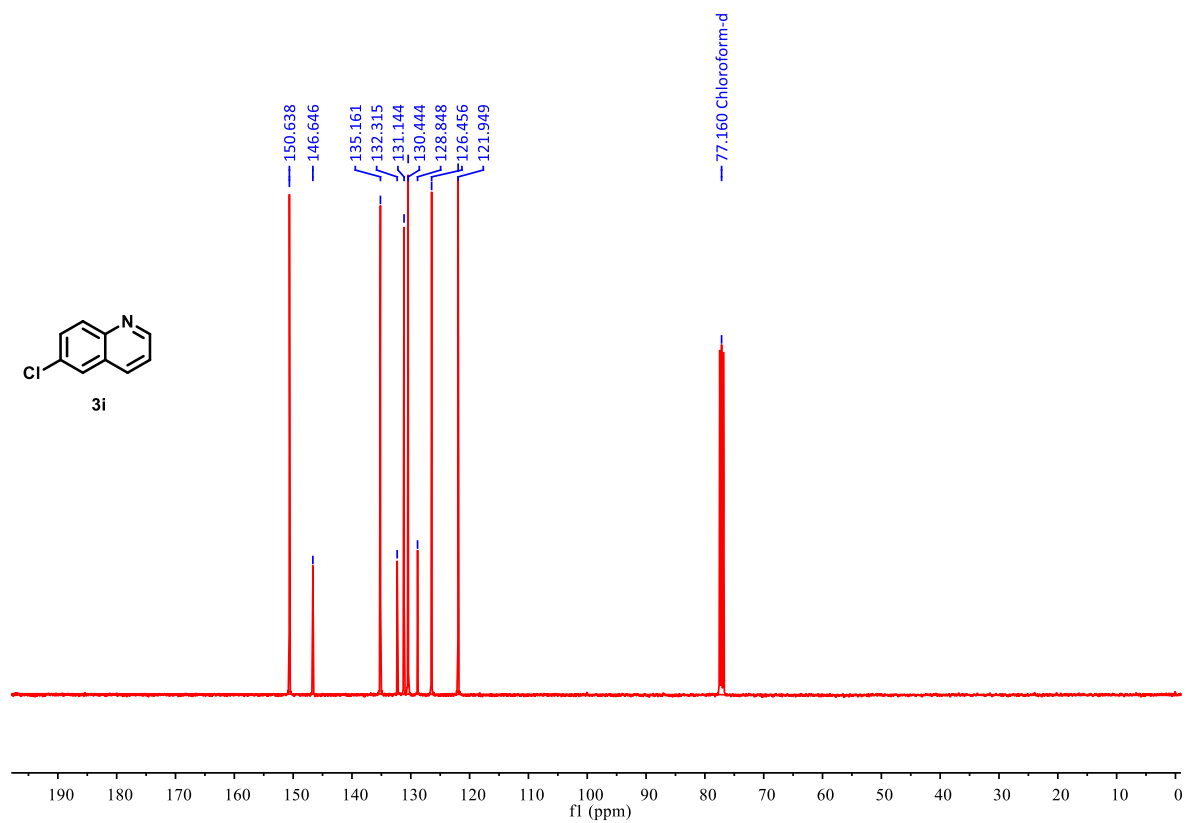


6-chloroquinoline(3i):

¹H NMR, 400 MHz, CDCl₃

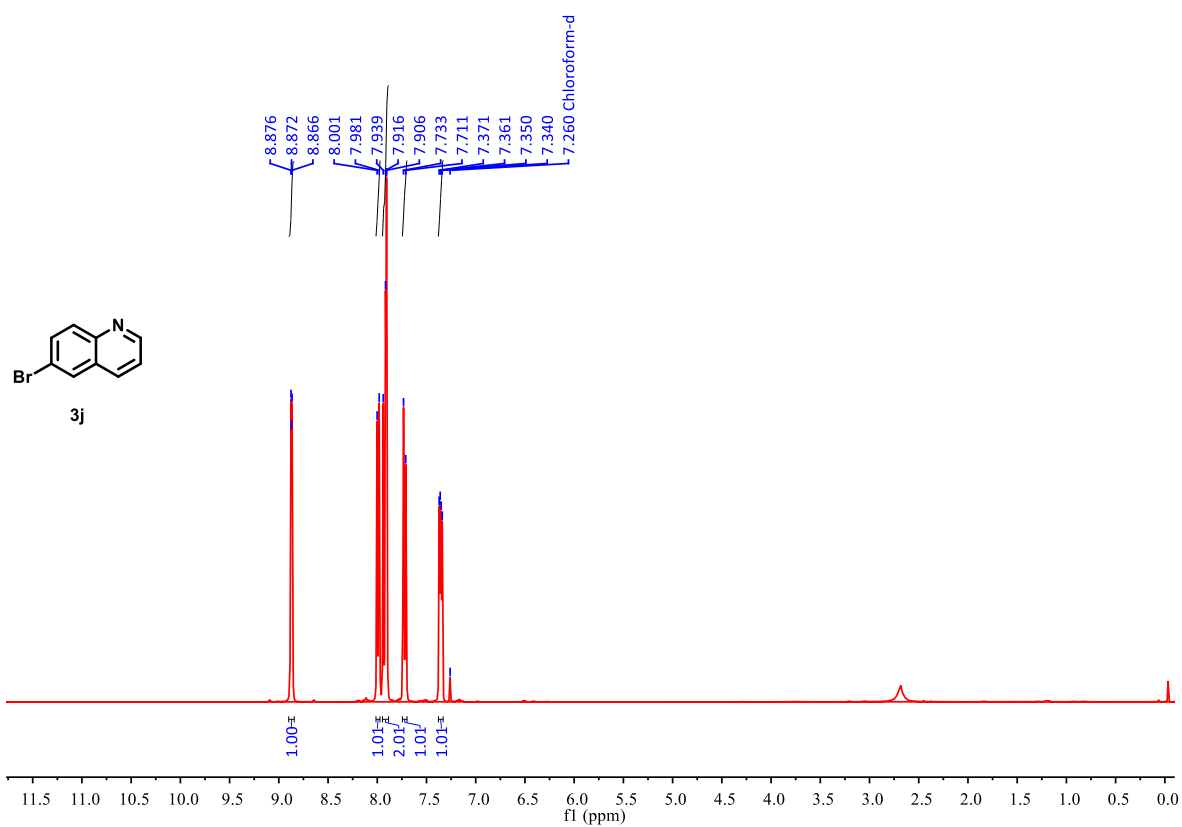


¹³C NMR, 101 MHz, CDCl₃

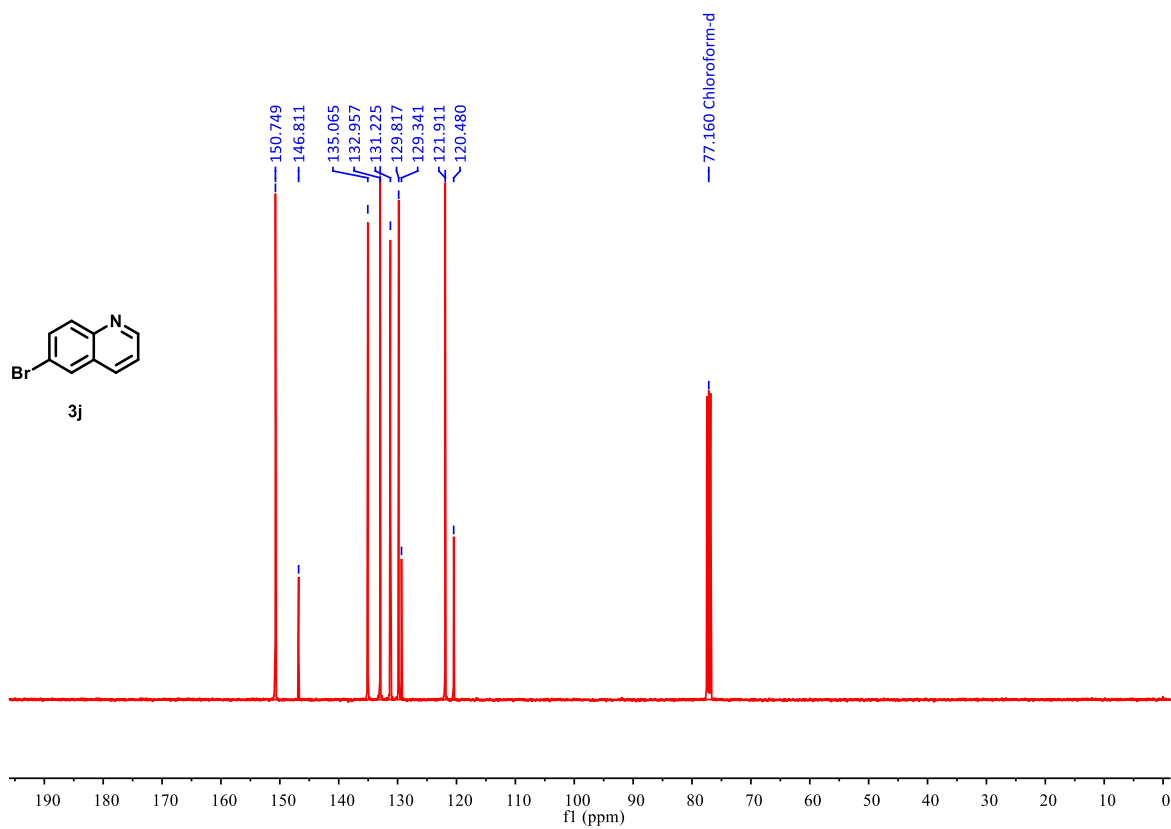


6-bromoquinoline(3j):

¹H NMR, 400 MHz, CDCl₃

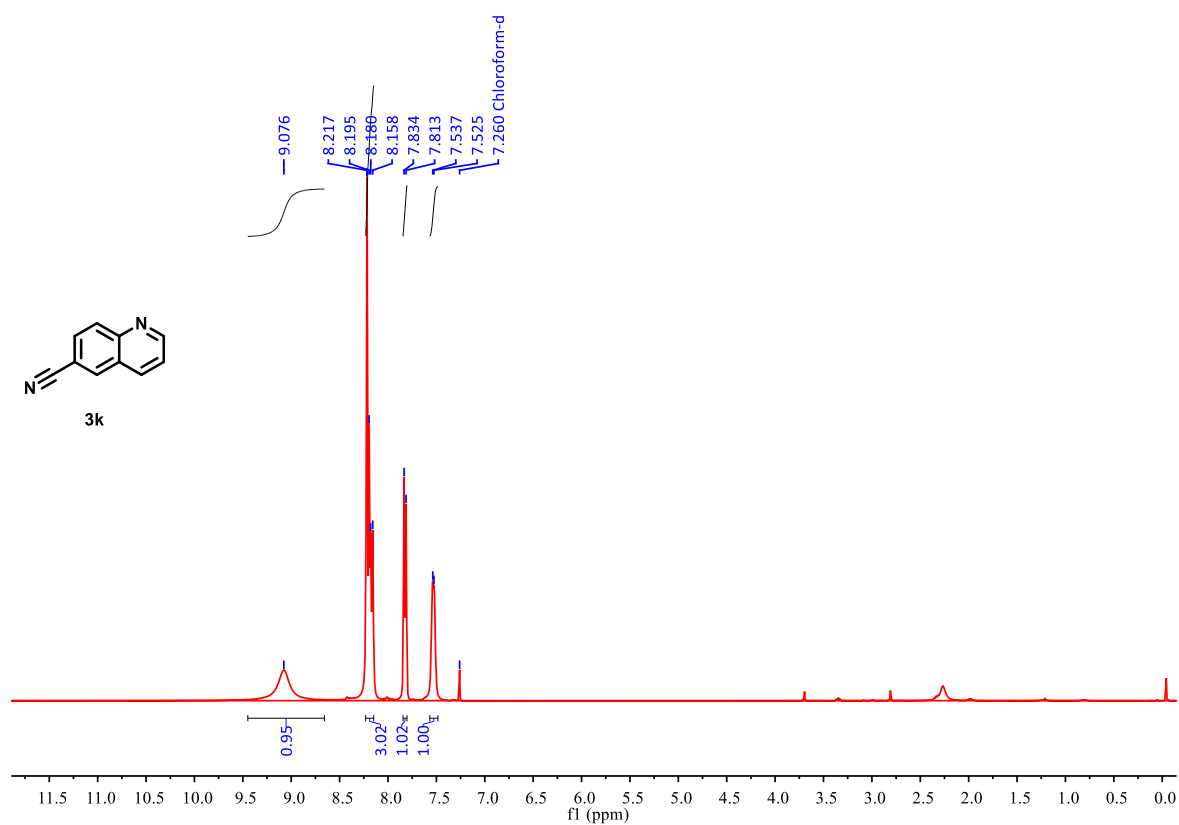


¹³C NMR, 101 MHz, CDCl₃

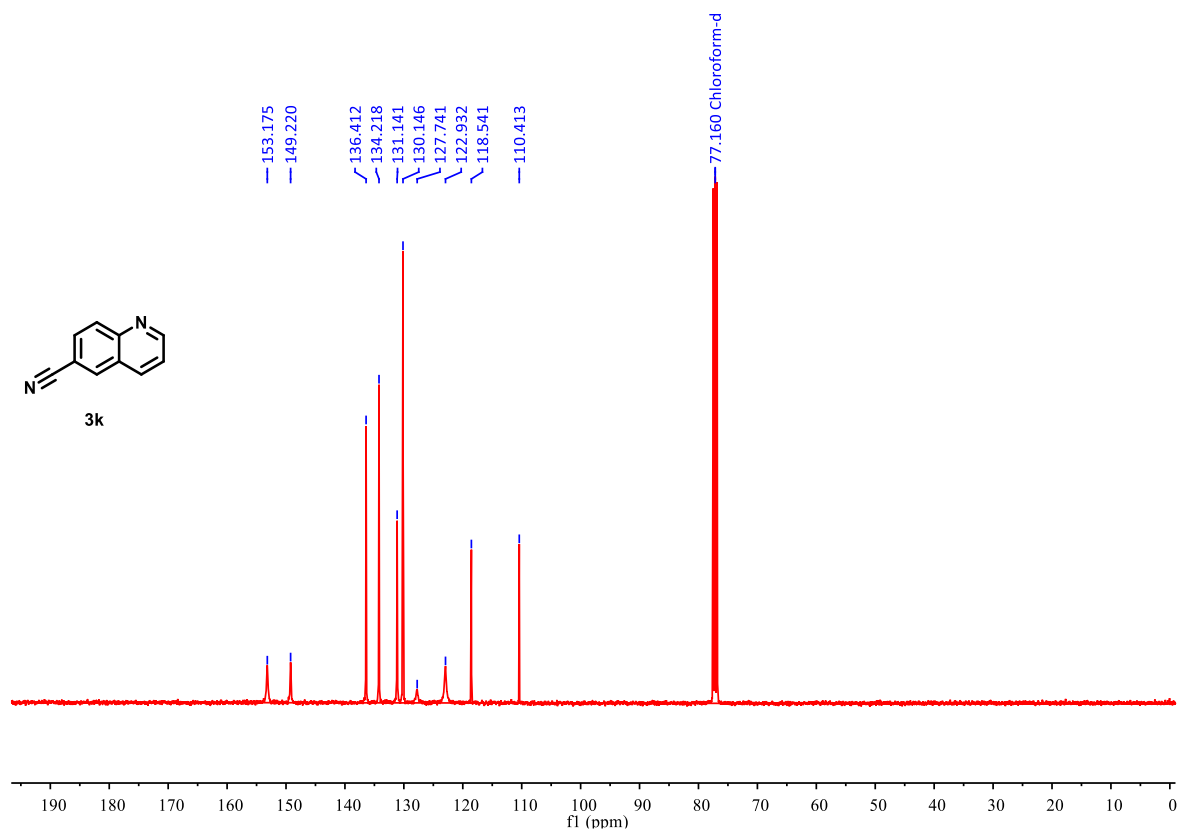


quinoline-6-carbonitrile(3k):

¹H NMR, 400 MHz, CDCl₃

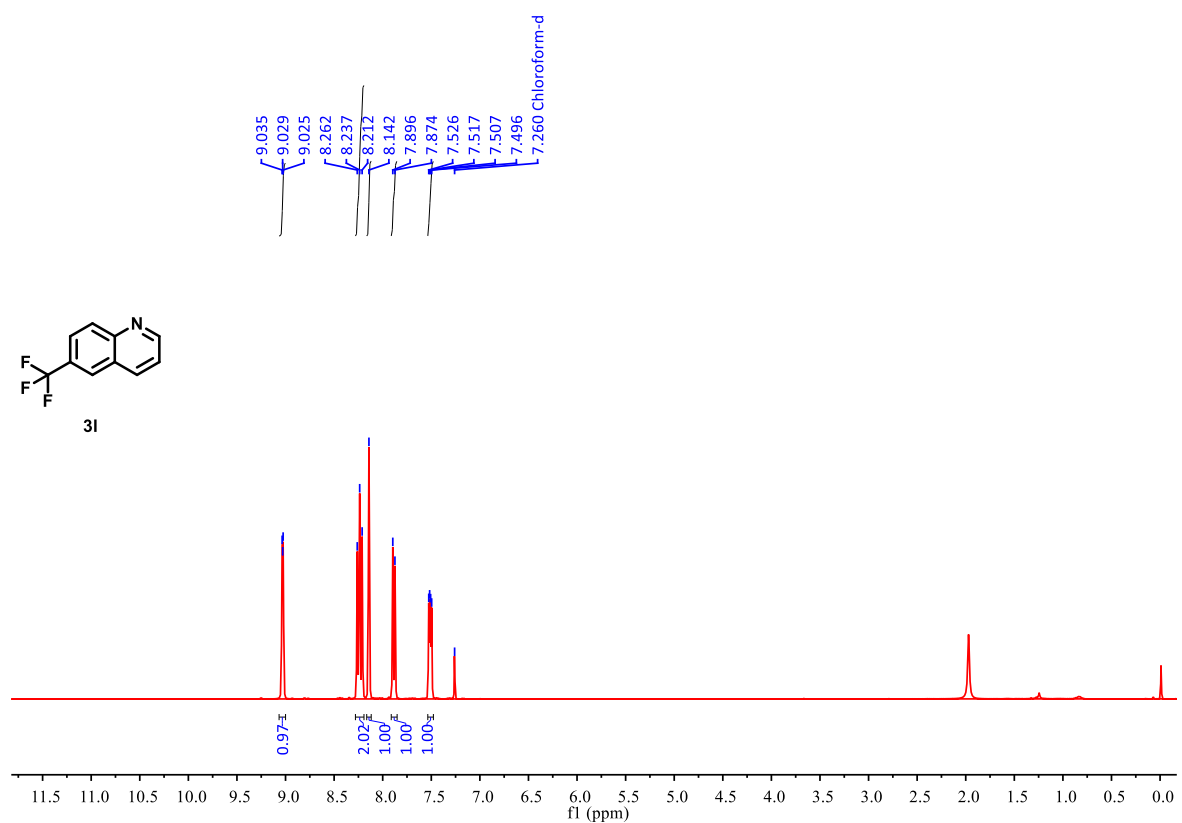


¹³C NMR, 101 MHz, CDCl₃

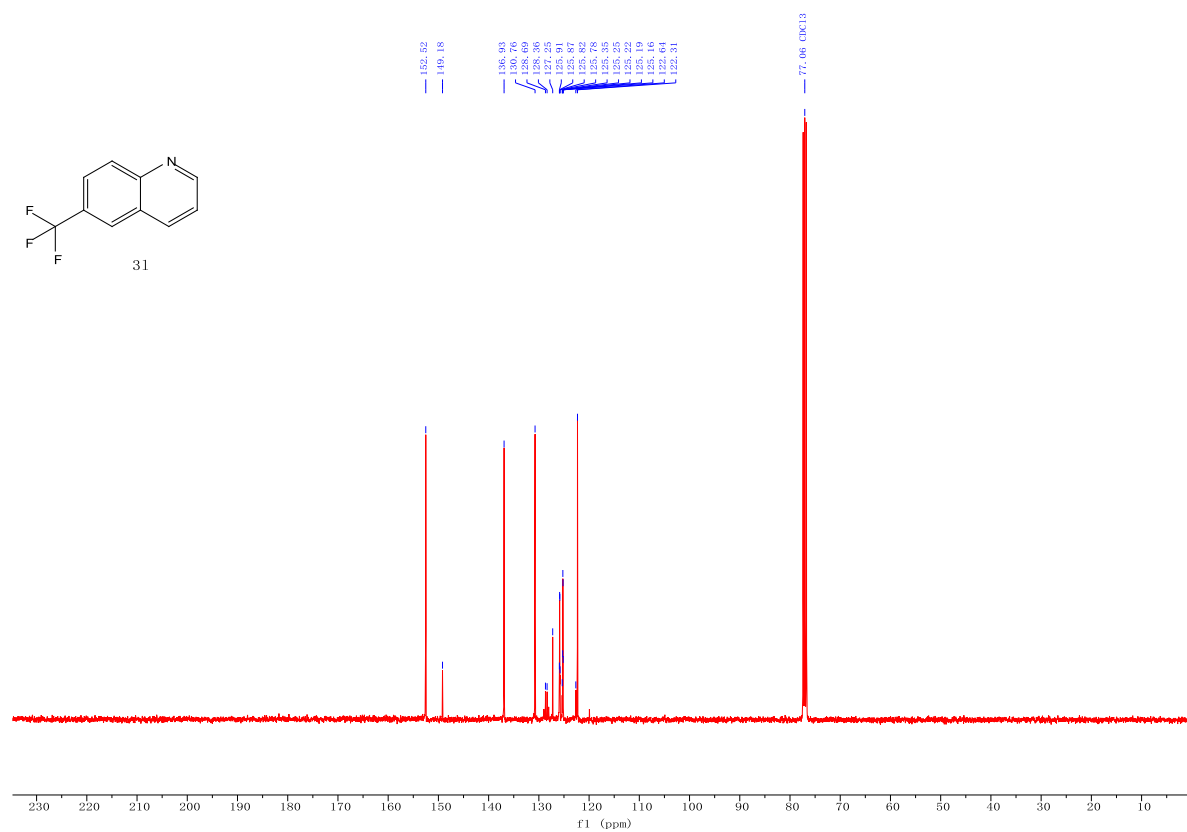


6-(trifluoromethyl)quinoline(3l):

¹H NMR, 400 MHz, CDCl₃

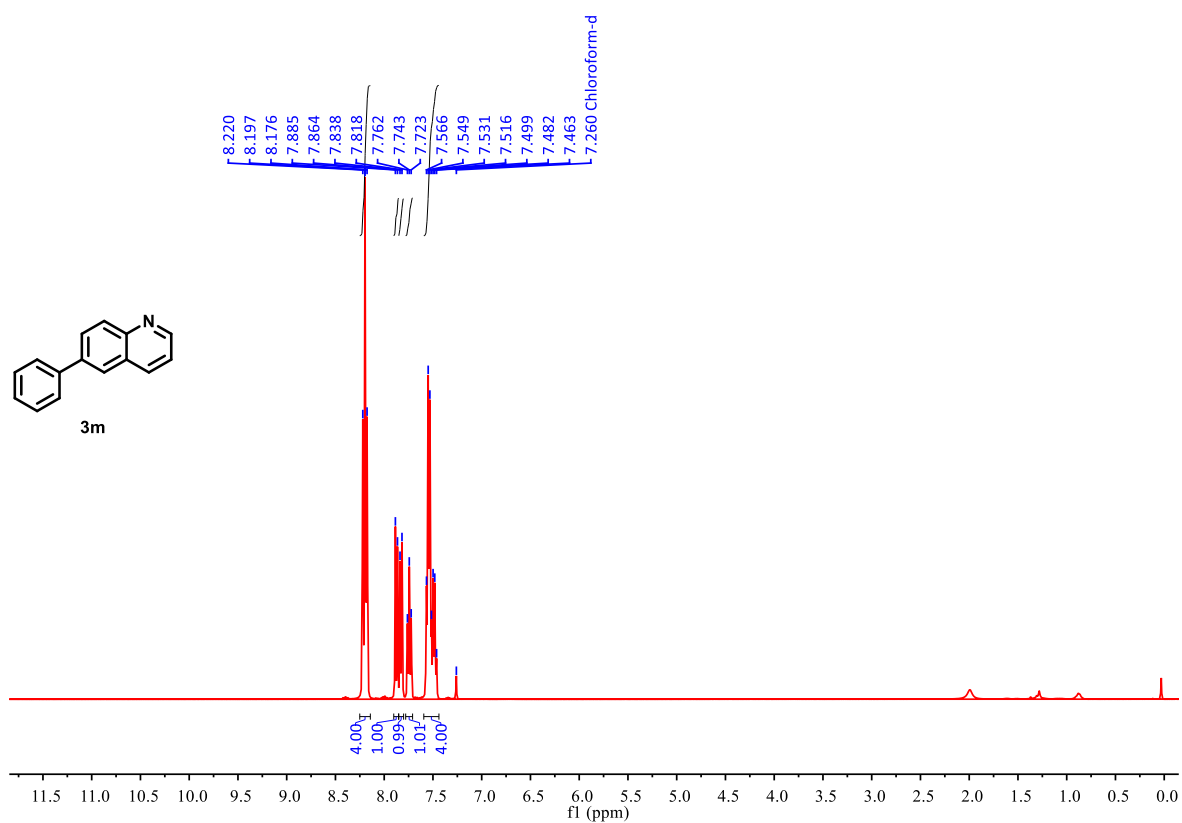


¹³C NMR, 101 MHz, CDCl₃

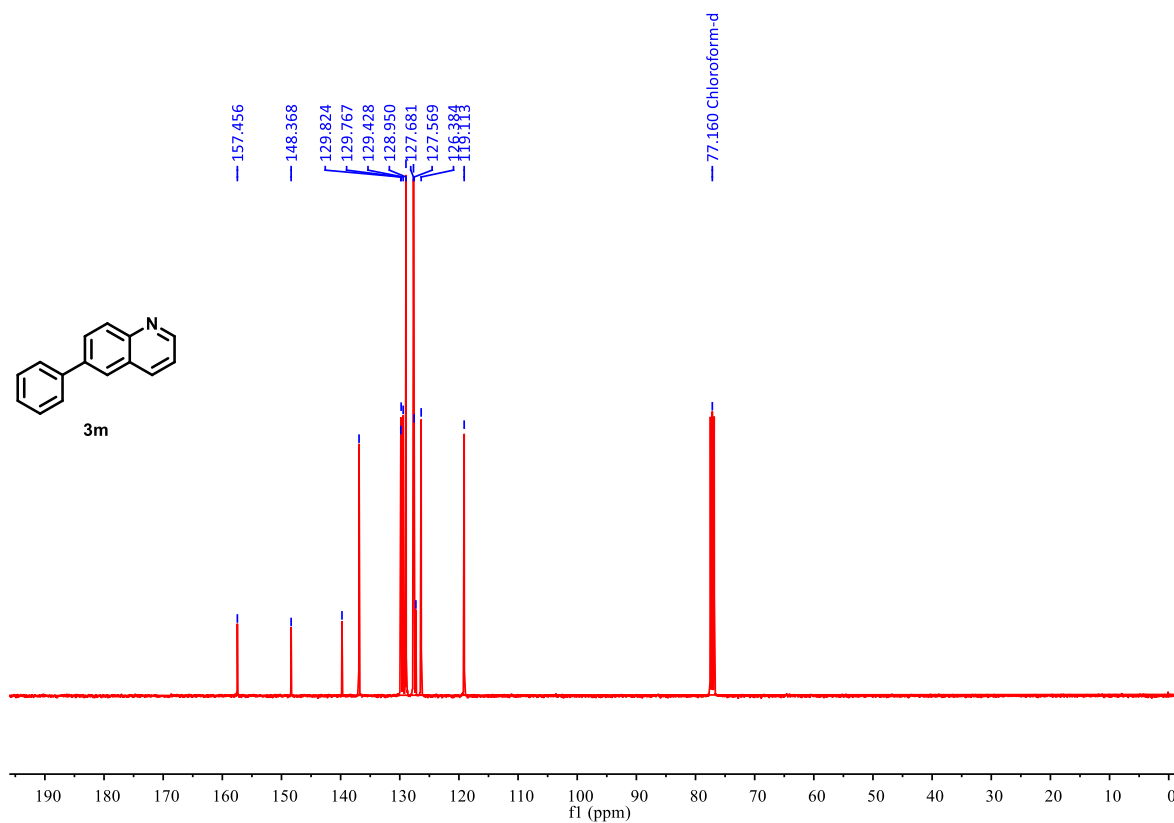


6-phenylquinoline(3m):

¹H NMR, 400 MHz, CDCl₃

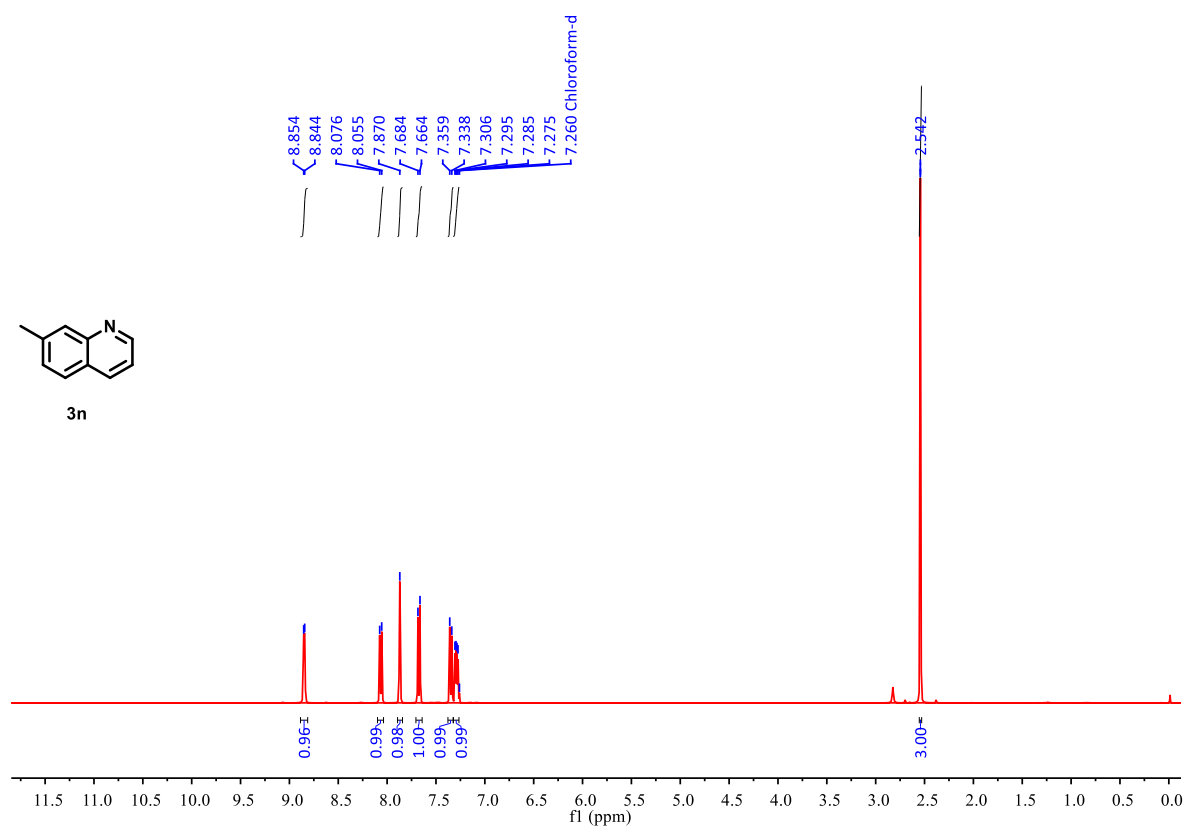


¹³C NMR, 101 MHz, CDCl₃

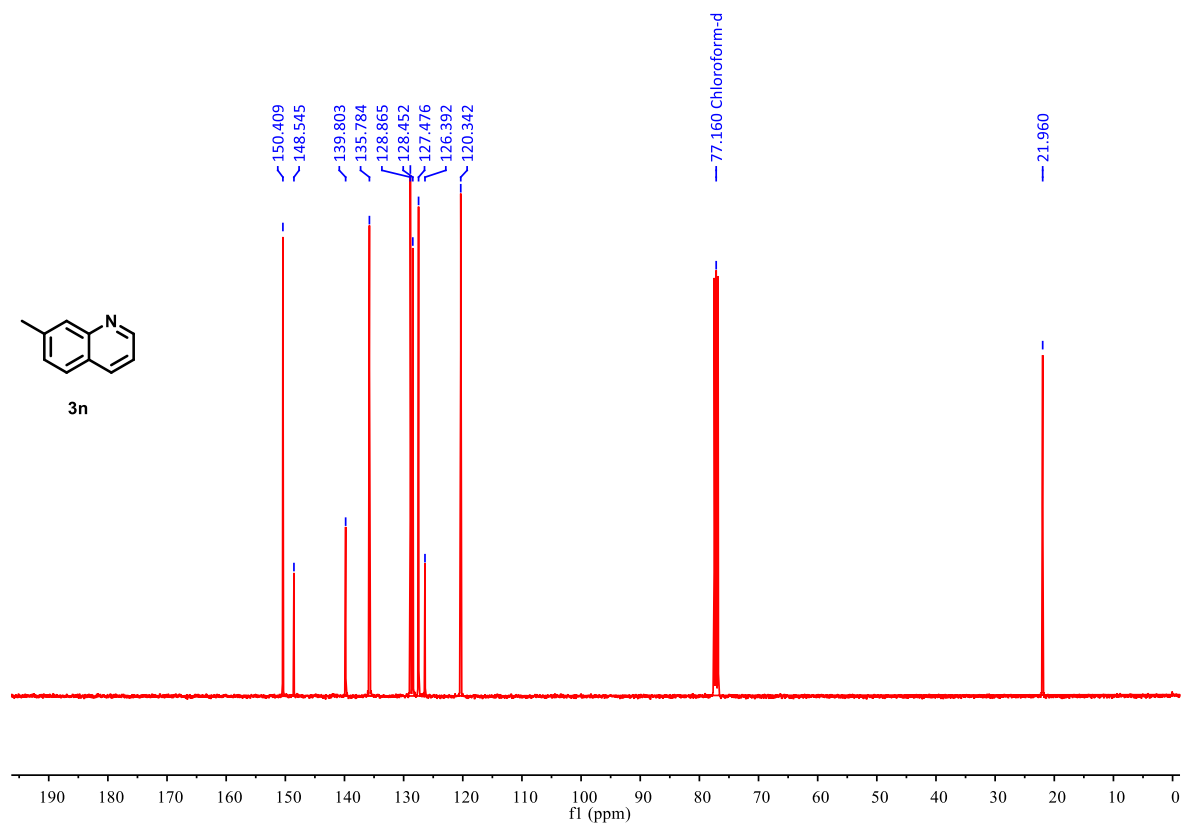


7-methylquinoline(3n):

¹H NMR, 400 MHz, CDCl₃

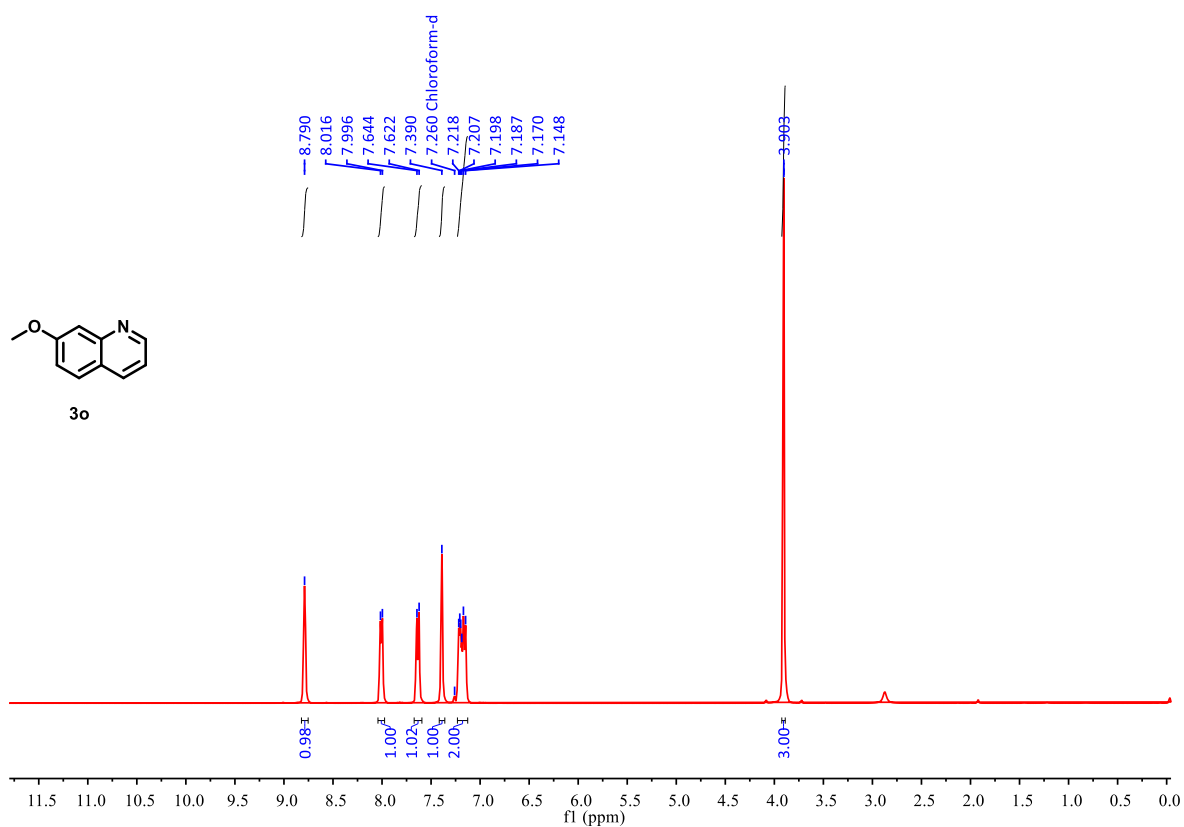


¹³C NMR, 101 MHz, CDCl₃

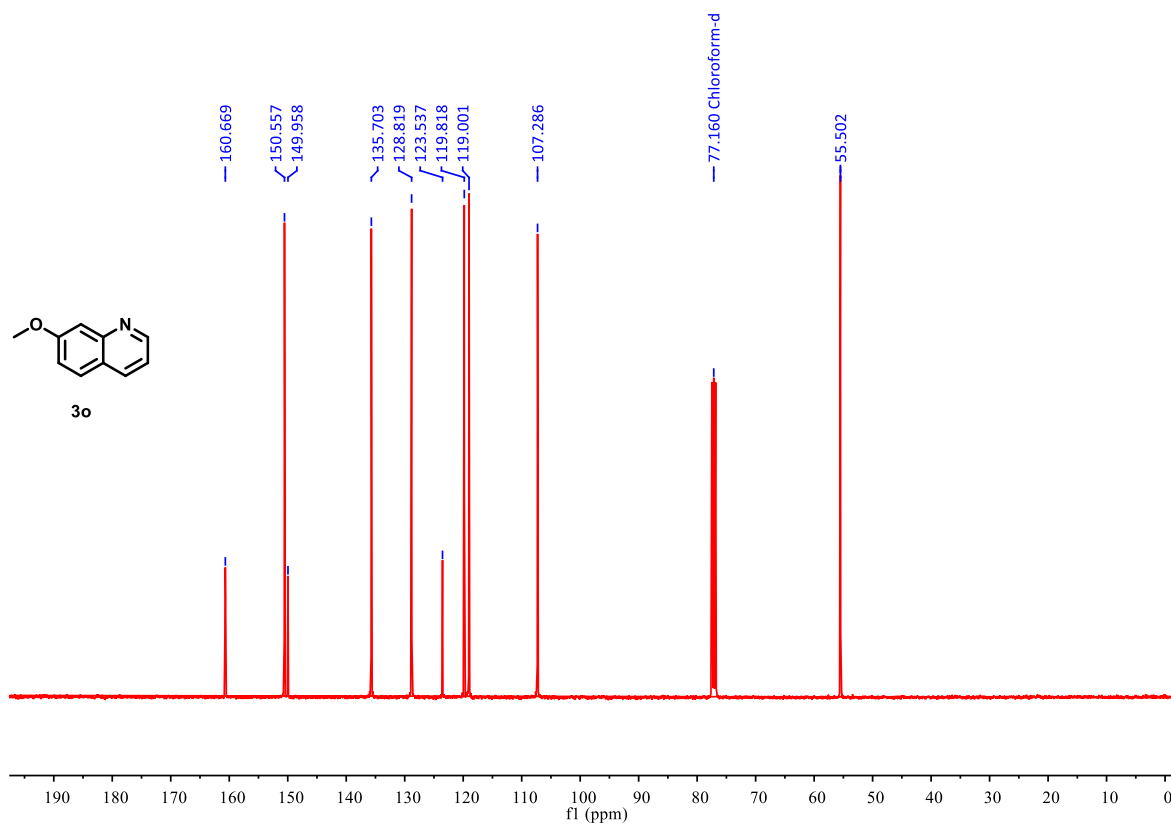


7-methoxyquinoline(3o):

¹H NMR, 400 MHz, CDCl₃

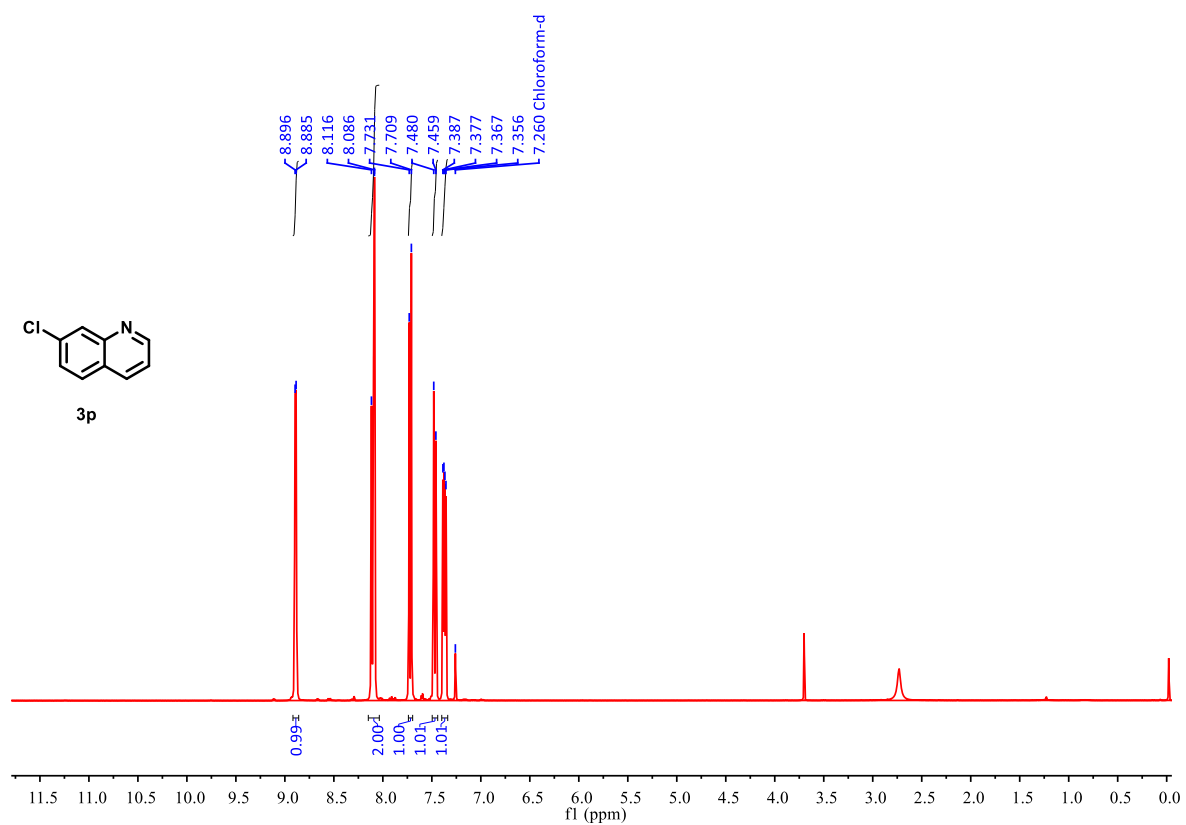


¹³C NMR, 101 MHz, CDCl₃

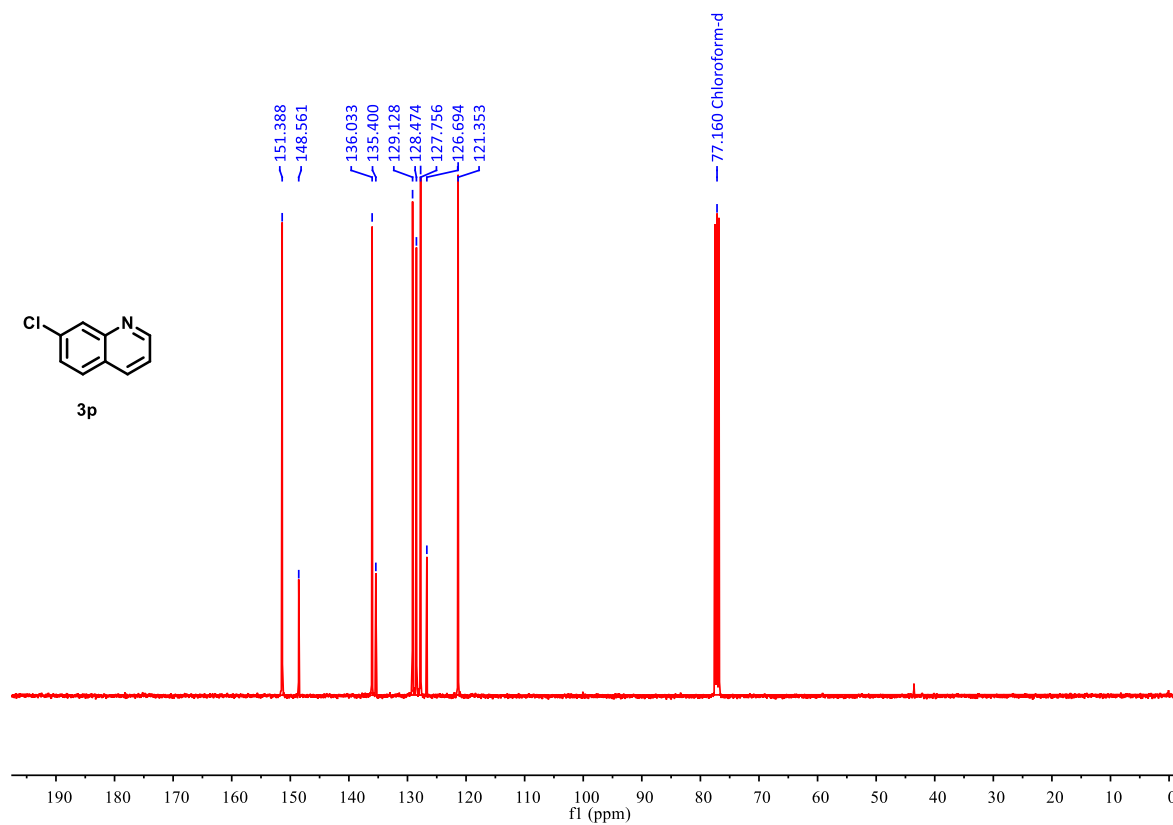


7-chloroquinoline(3p):

¹H NMR, 400 MHz, CDCl₃

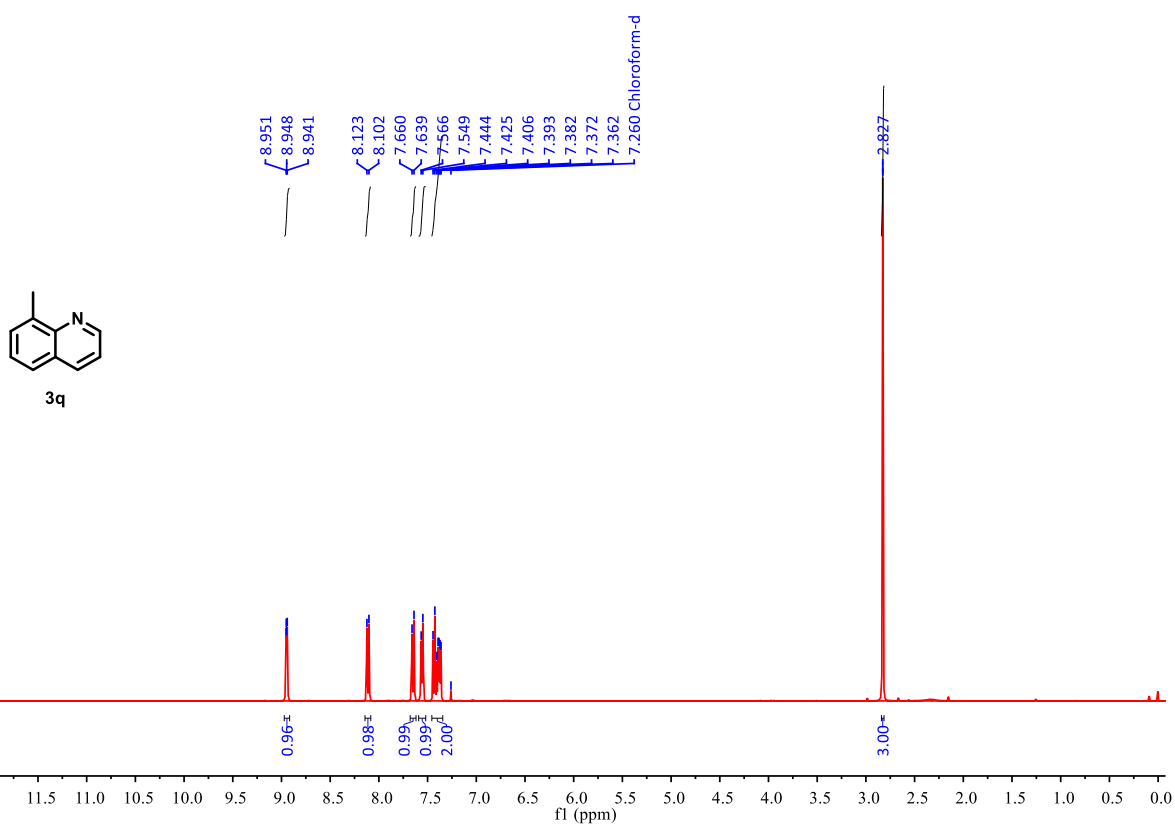


¹³C NMR, 101 MHz, CDCl₃

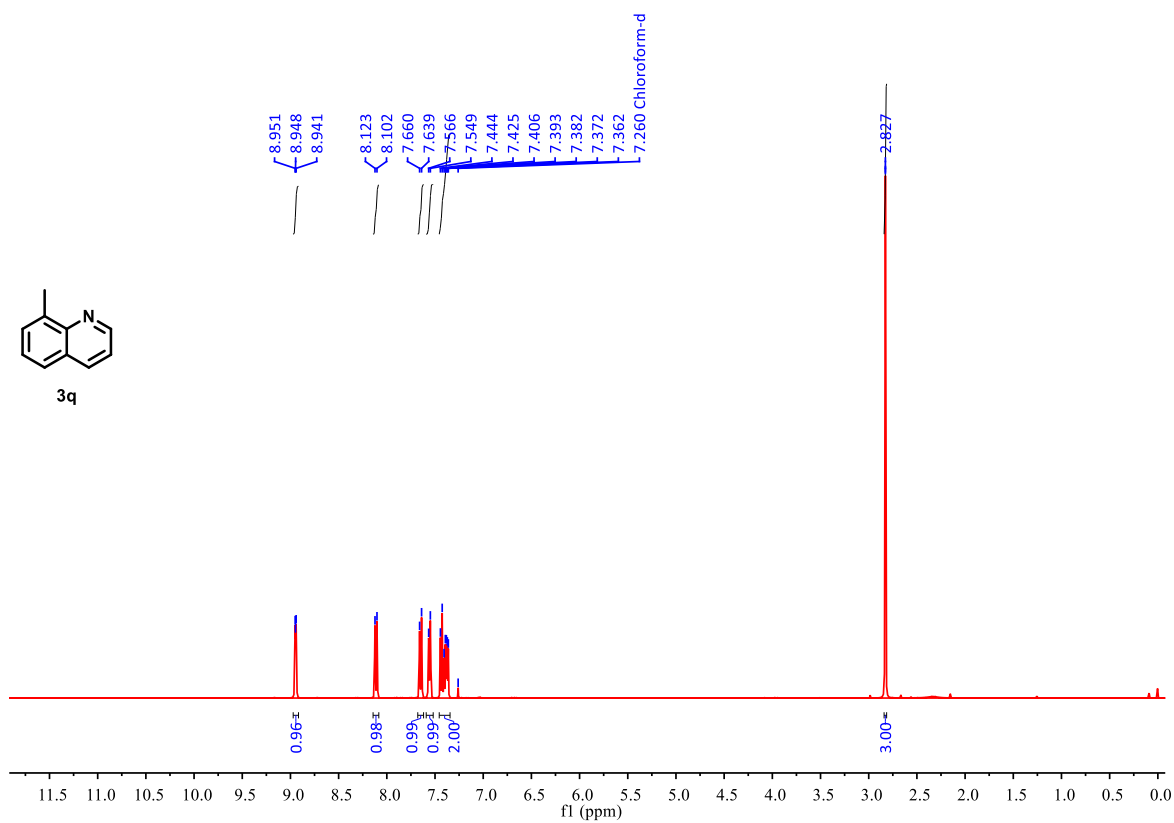


8-methylquinoline(3q):

¹H NMR, 400 MHz, CDCl₃

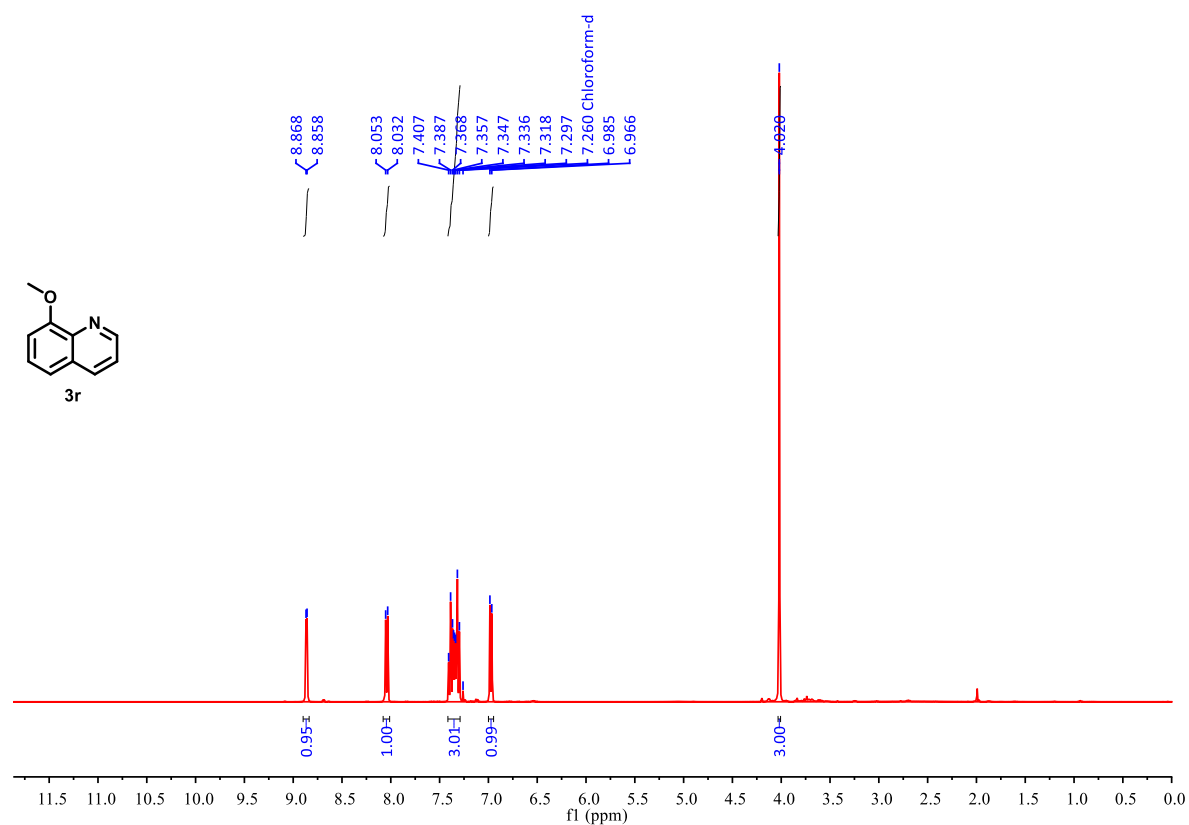


¹³C NMR, 101 MHz, CDCl₃

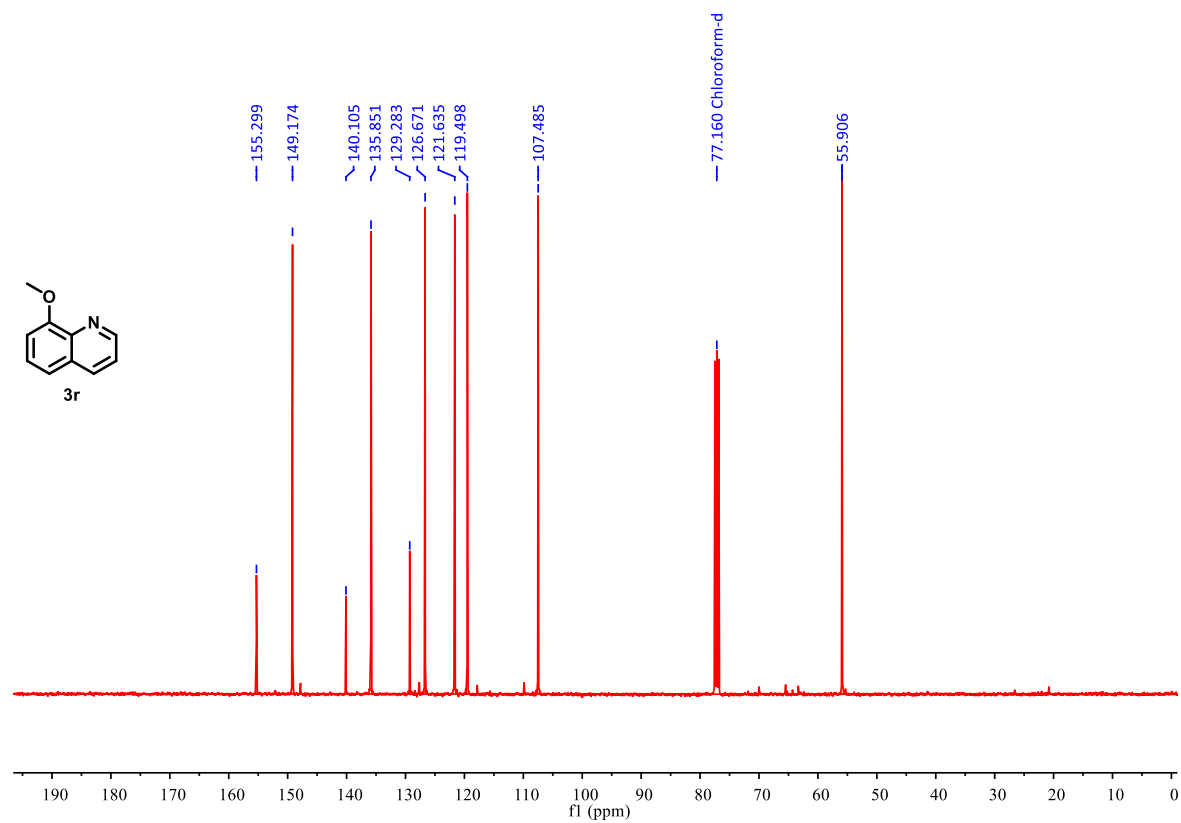


8-methoxyquinoline(3r):

¹H NMR, 400 MHz, CDCl₃

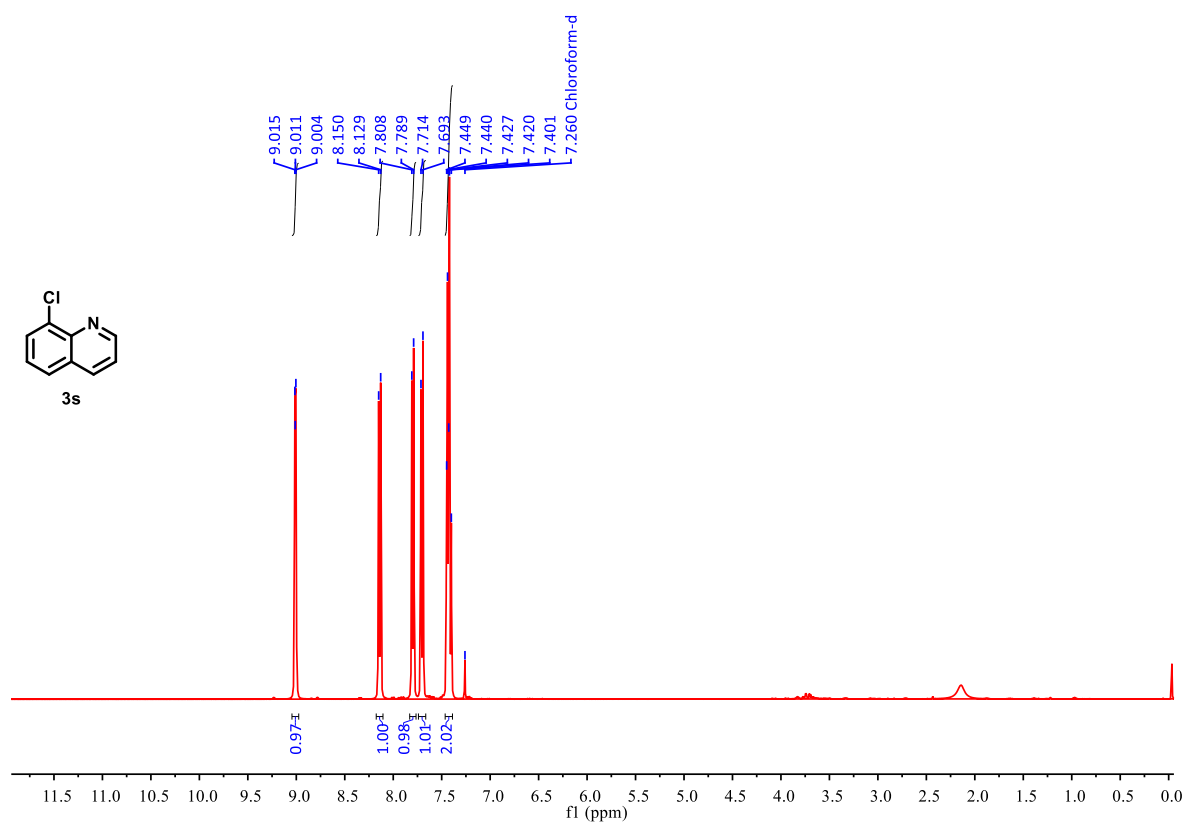


¹³C NMR, 101 MHz, CDCl₃

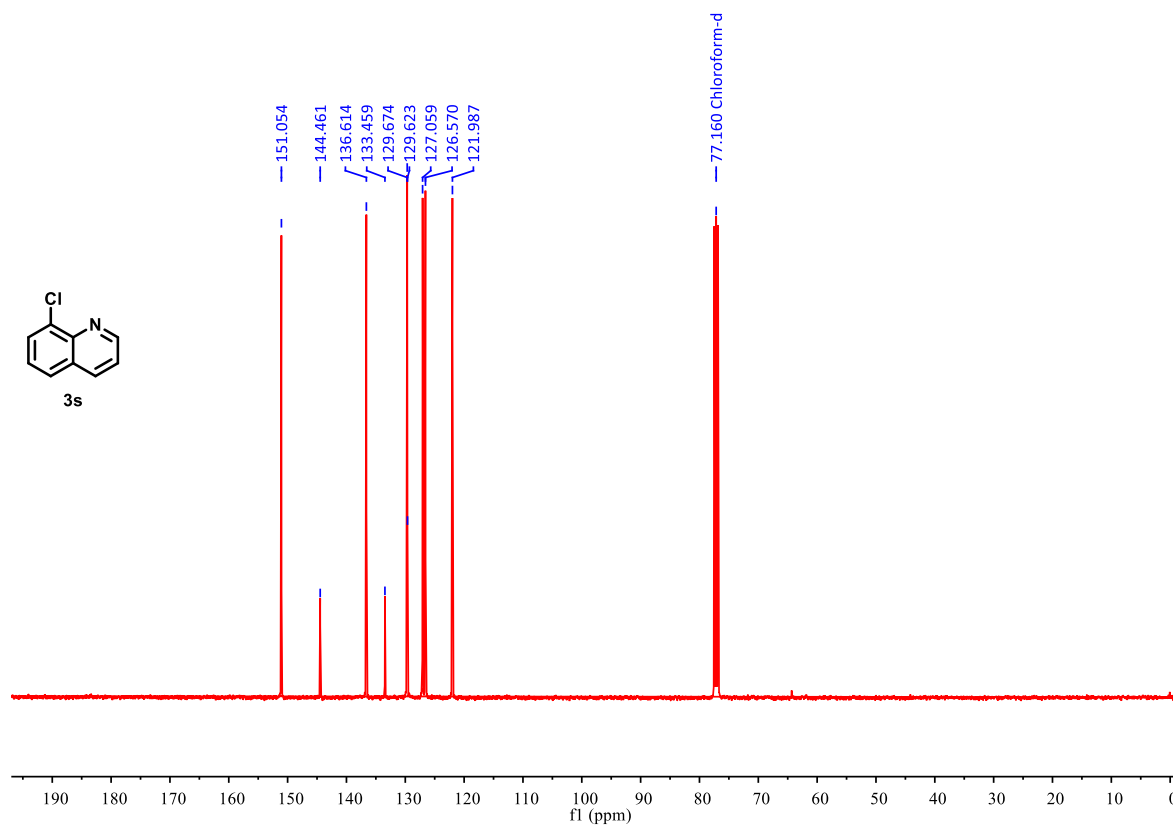


8-chloroquinoline(3s):

¹H NMR, 400 MHz, CDCl₃

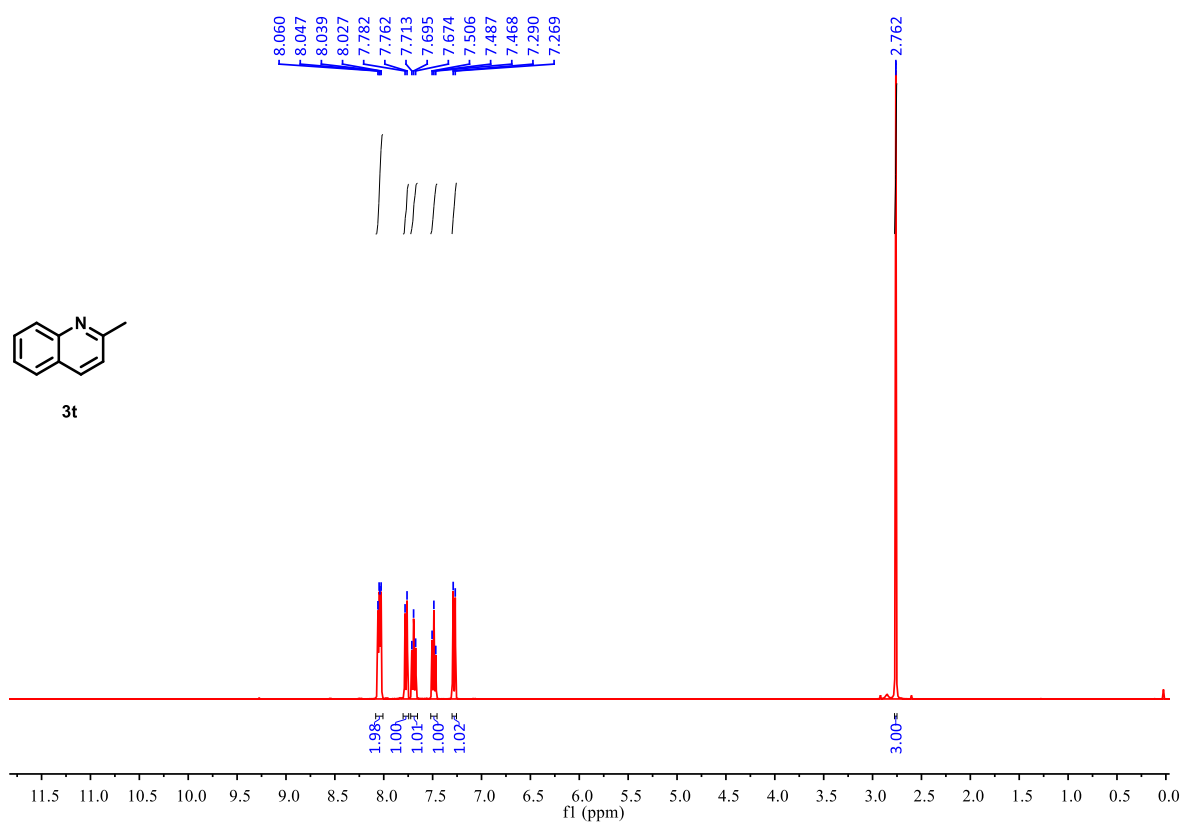


¹³C NMR, 101 MHz, CDCl₃

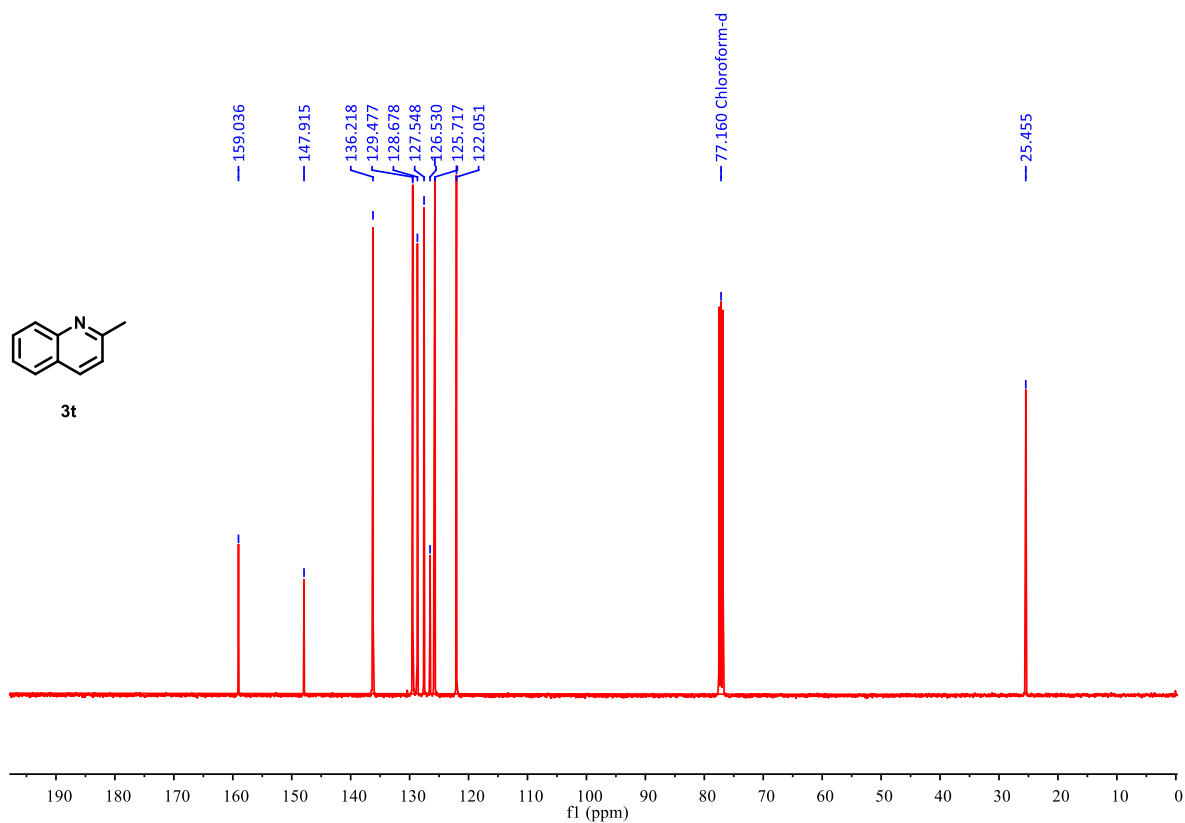


2-methylquinoline(3t):

¹H NMR, 400 MHz, CDCl₃

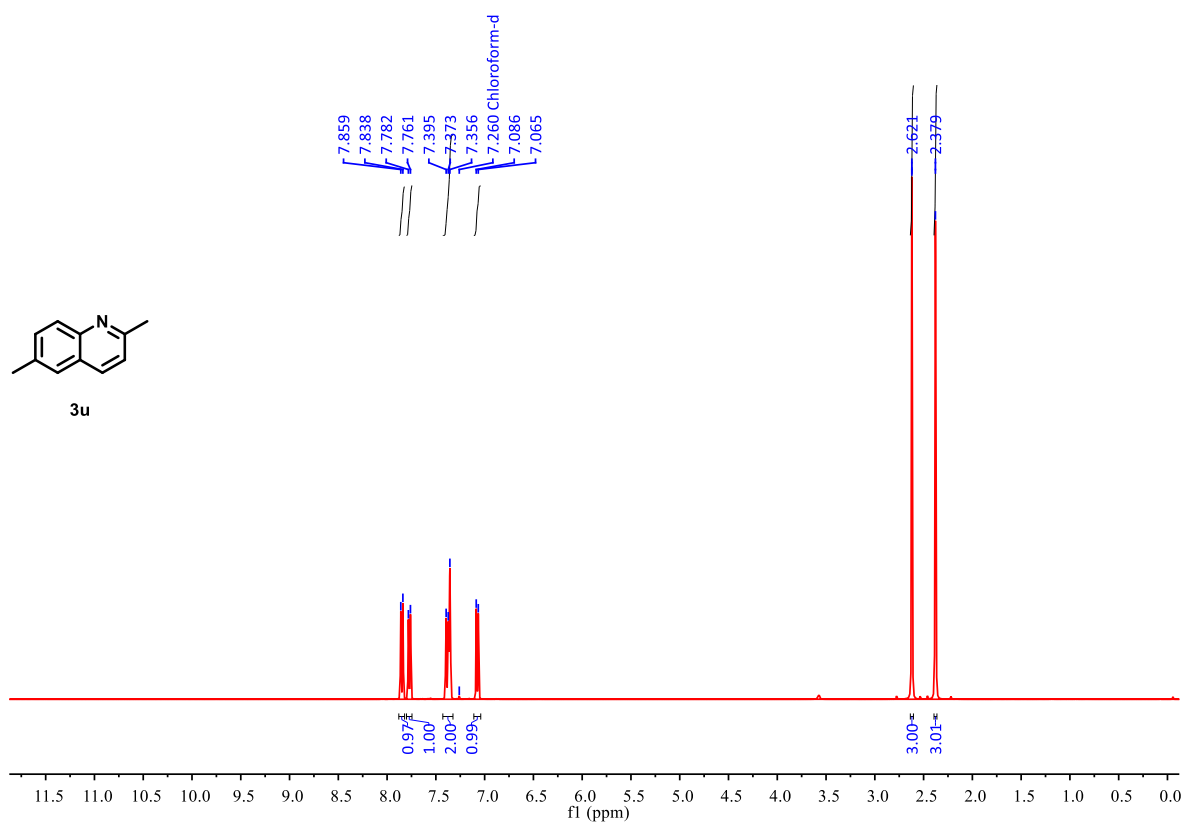


¹³C NMR, 101 MHz, CDCl₃

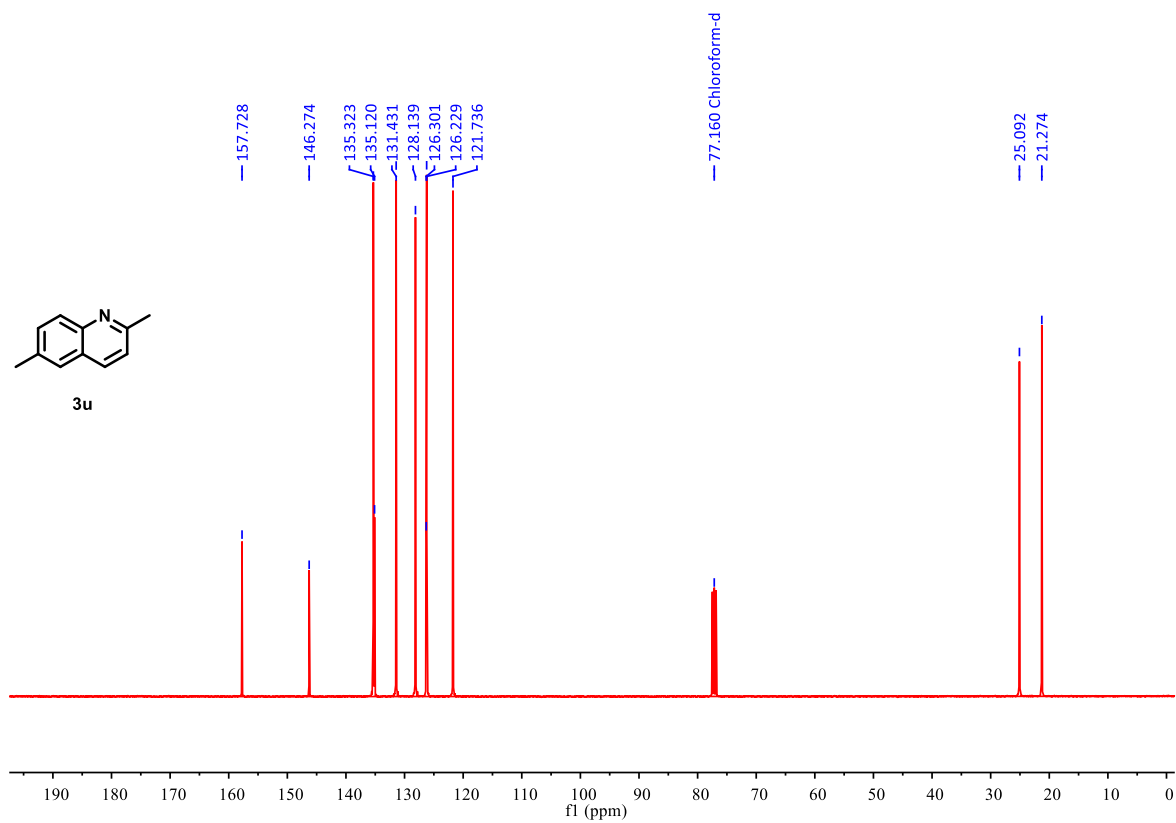


2,6-dimethylquinoline(3u):

¹H NMR, 400 MHz, CDCl₃

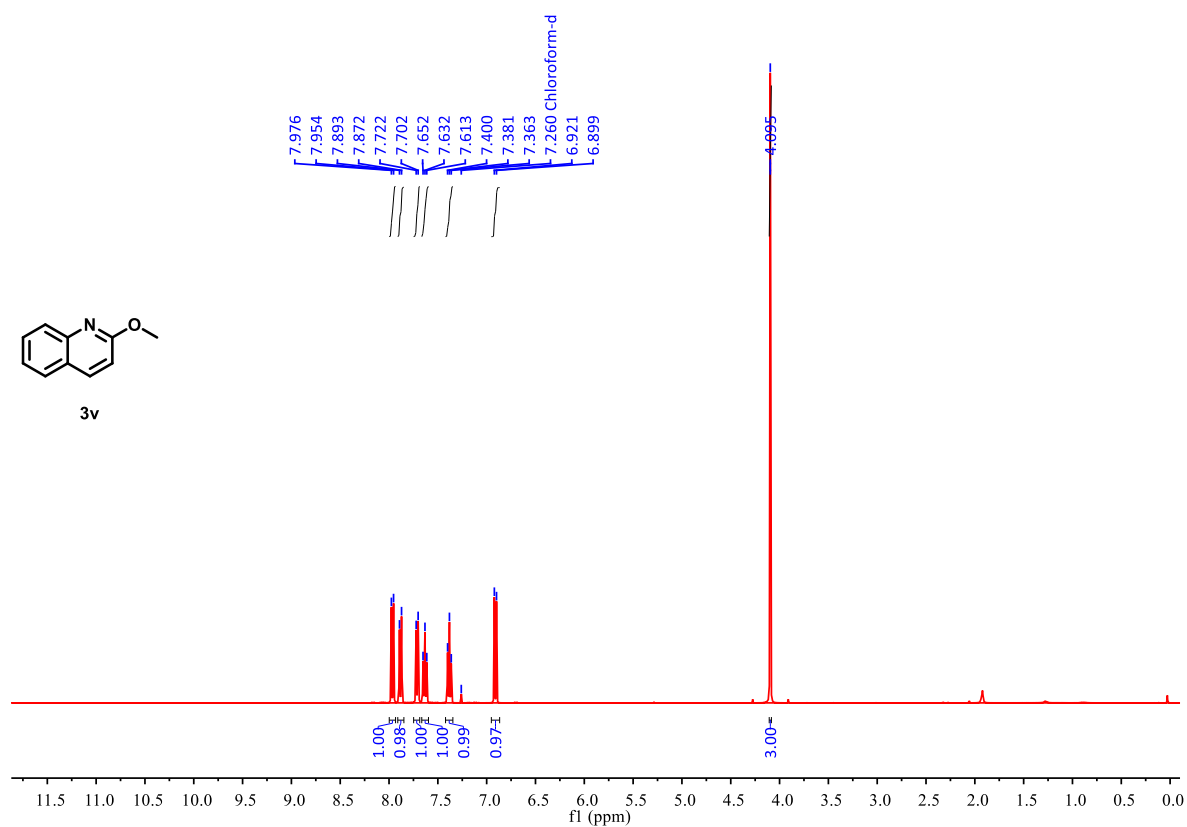


¹³C NMR, 101 MHz, CDCl₃

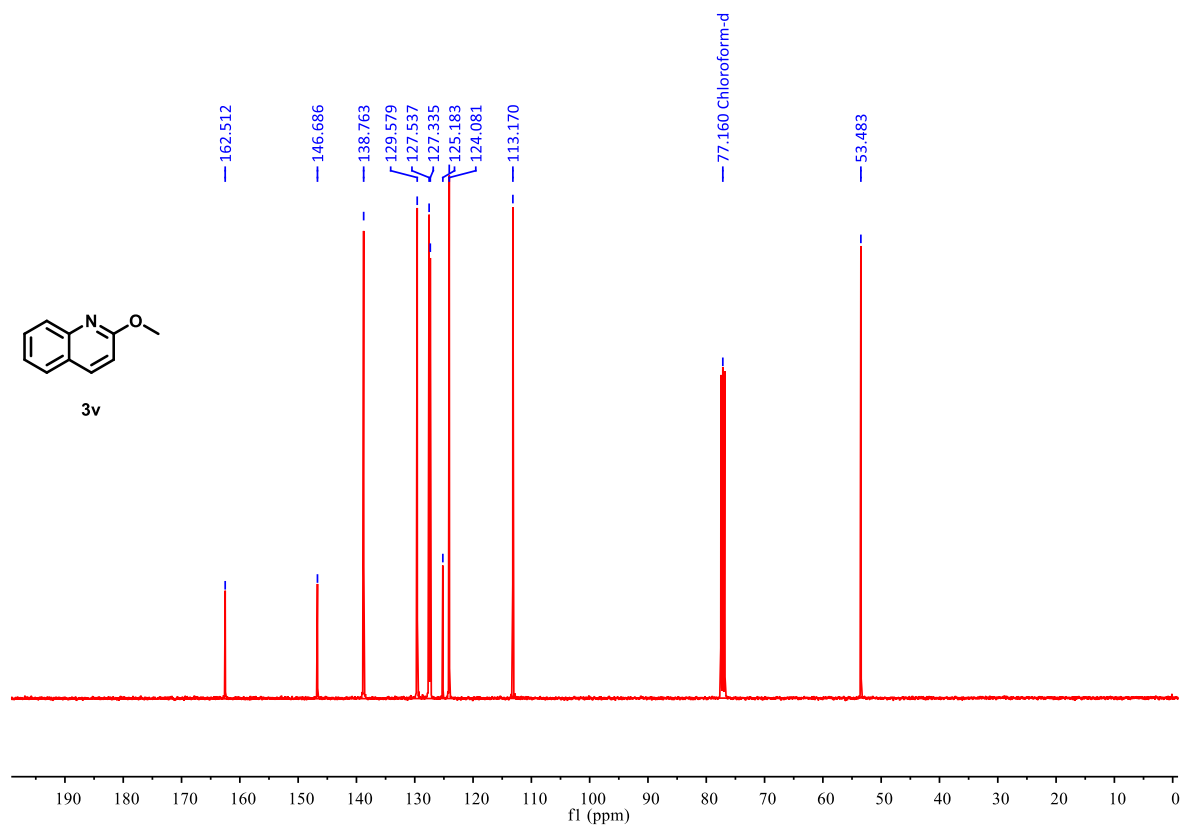


2-methoxyquinoline(3v):

¹H NMR, 400 MHz, CDCl₃

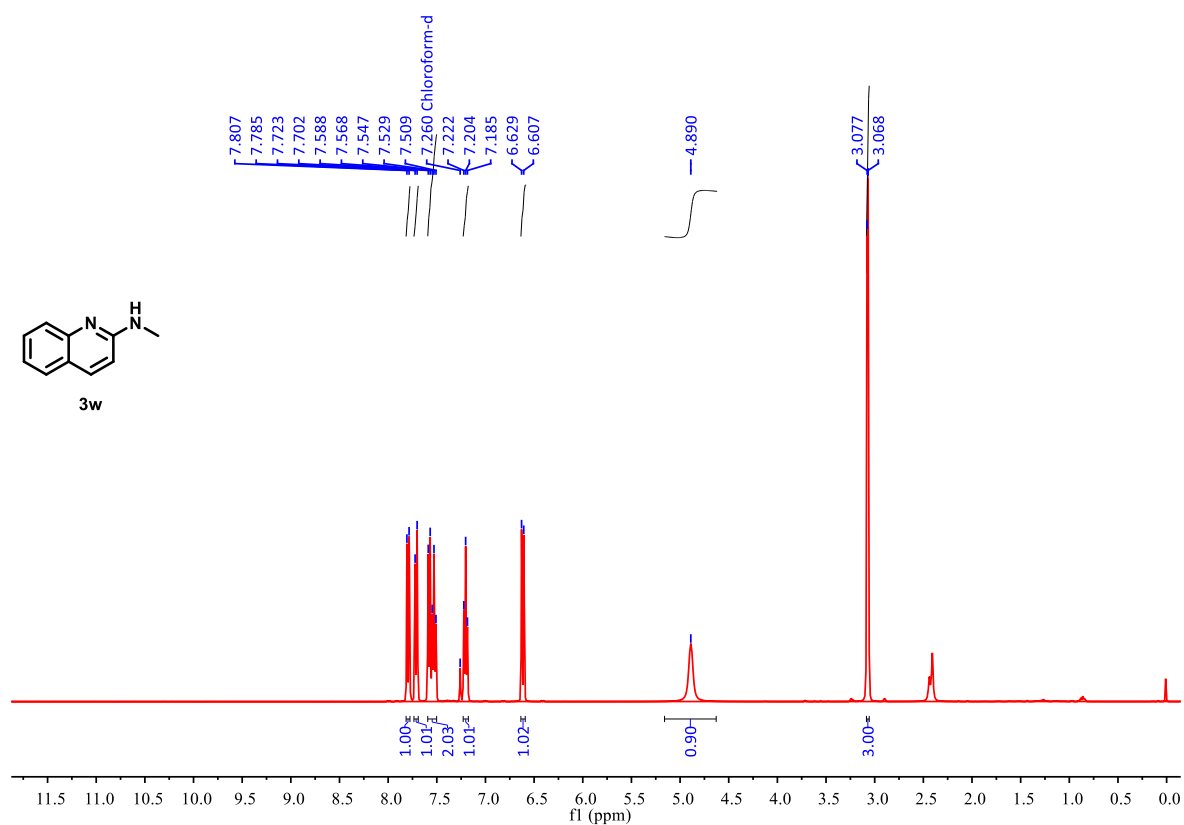


¹³C NMR, 101 MHz, CDCl₃

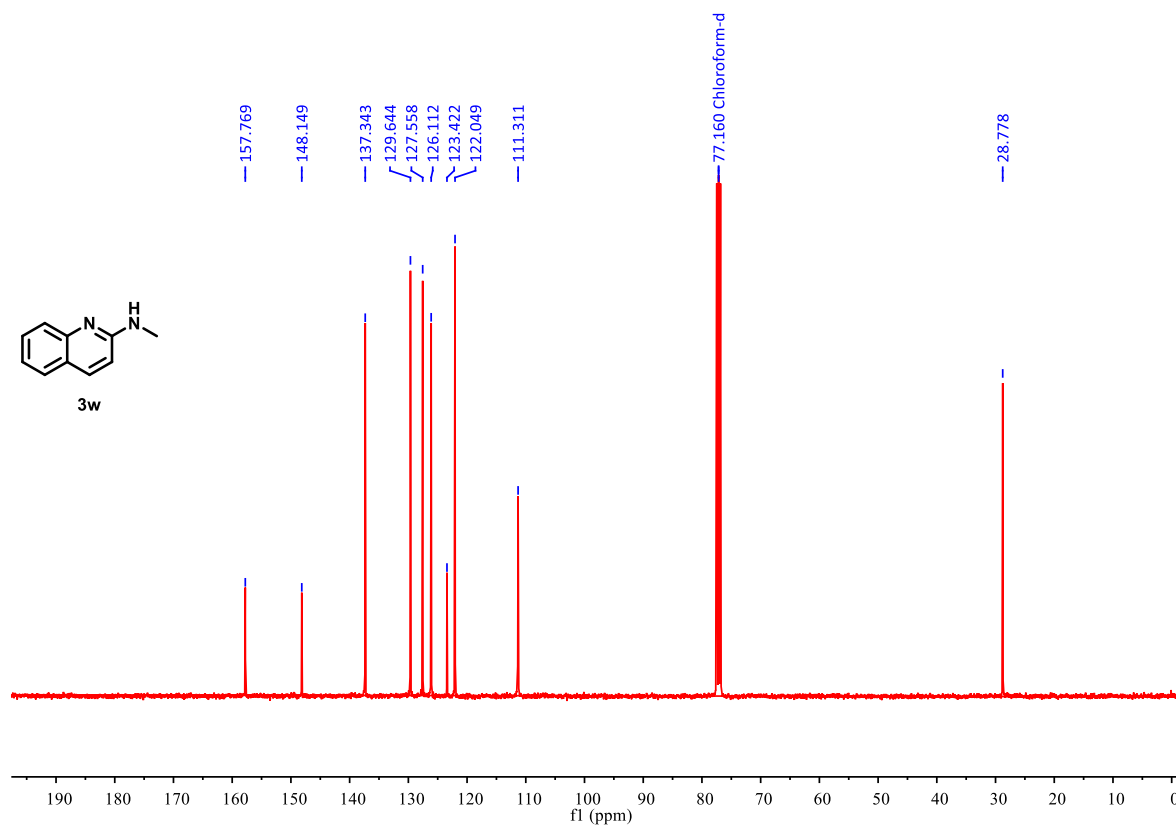


N-methylquinolin-2-amine(3w):

¹H NMR, 400 MHz, CDCl₃

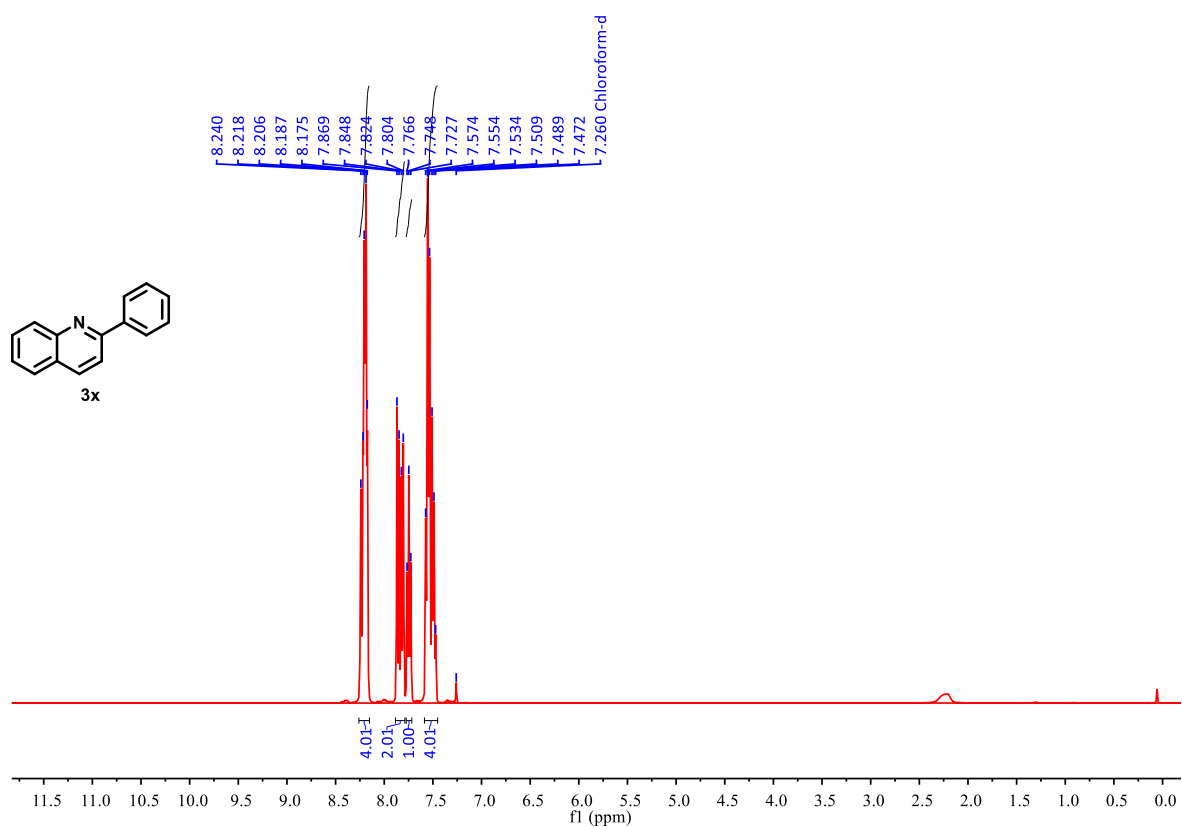


¹³C NMR, 101 MHz, CDCl₃

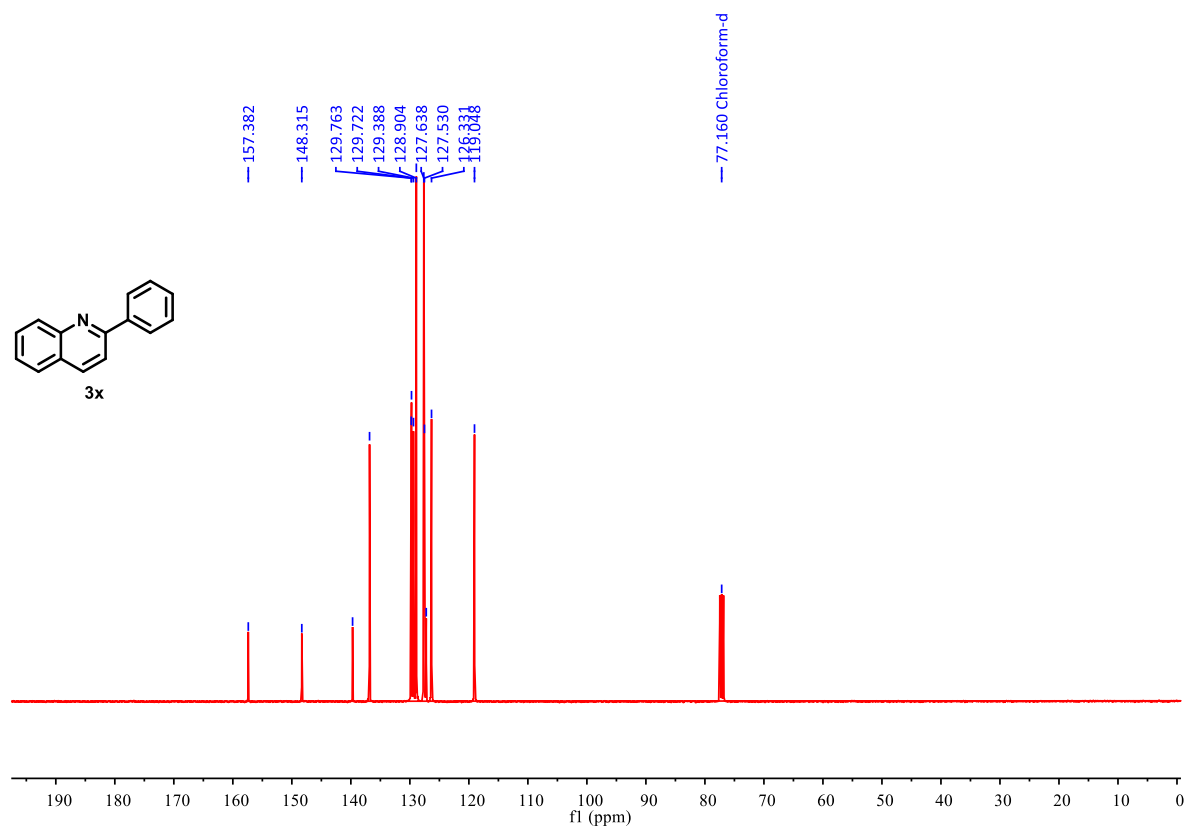


2-phenylquinoline(3x):

¹H NMR, 400 MHz, CDCl₃

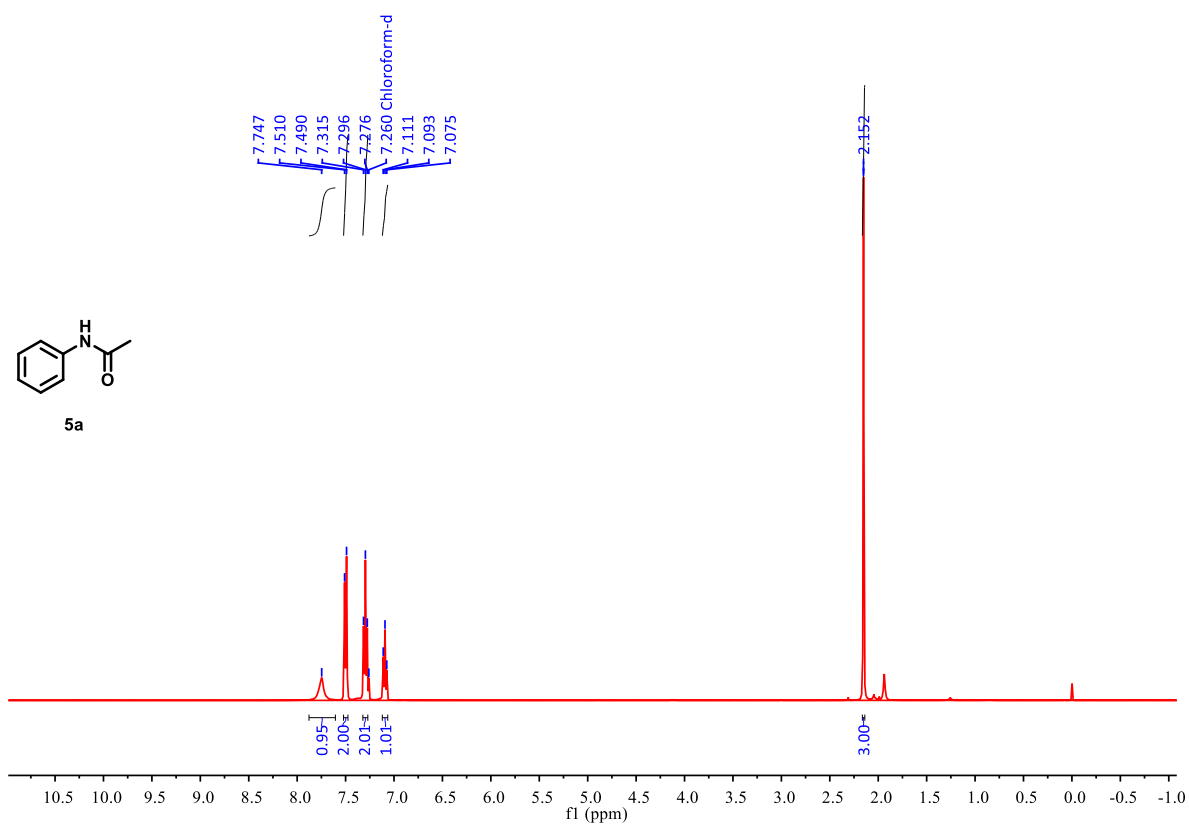


¹³C NMR, 101 MHz, CDCl₃



N-phenylacetamide(5a):

¹H NMR, 400 MHz, CDCl₃



¹³C NMR, 101 MHz, CDCl₃

